

# MATLAB SOLUTIONS TO THE CHEMICAL ENGINEERING PROBLEM SET

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## INTRODUCTION

These solutions are for a set of numerical problems in chemical engineering. The problems were developed by Professor Michael B. Cutlip of the University of Connecticut and Professor Mordechai Shacham of Ben-Gurion University of the Negev for the ASEE Chemical Engineering Summer School held in Snowbird, Utah in August, 1997. The problem statements are provided in another document.<sup>1</sup> Professors Cutlip and Shacham provided a document which shows how to solve the problems using POLYMATH, Professor Eric Nuttall of the University of New Mexico provided solutions using Mathematica and Professor J. J. Hwalek provided solutions using Mathcad. After the conference, Professor Ross Taylor provided solutions in Maple, and Edward Rosen provided solutions in EXCEL. This paper gives the solution in MATLAB. All documents and solutions are available from <http://www.che.utexas/cache>.

These solutions are obtained using the version 5.0 of MATLAB Pro. Minor changes are needed to the files when using version 4.0 of MATLAB, mainly in the command giving the limits of integration when solving ordinary differential equations. The appropriate commands (changes from MATLAB 5.0) are given in the files as comments. The program MATLAB runs by executing commands, which can call files called m-files. Given below are the commands and m-files. The m-files are also available on a diskette. For ease in interpreting the text below, text is printed in Times font, whereas the MATLAB files are printed in Geneva font. Each problem is solved by setting the path for MATLAB (most easily done by opening the appropriate m-file, and issuing the command Prob\_X. The m-file Prob\_X.m may call other m-files, which are described below and are on the diskette. In the description below, any line beginning with a % is a comment.

The authors thank Professor Larry Ricker for helpful comments on the first draft of this paper.

<sup>1</sup> Copyright by the authors, 1997. Material can be copied for educational purposes in chemical engineering departments. Otherwise permission must be obtained from the authors.

<sup>2</sup> Joseph Brule just obtained his B.S. degree. Tae Han is a current undergraduate. Dr. John Widmann a recent Ph.D. graduate, and Bruce Finlayson is the Rehrberg Professor and Chair.

<sup>3</sup> "The Use of Mathematical Software packages in Chemical Engineering", Michael B. Cutlip, John J. Hwalek, Eric H. Nuttall, Mordechai Shacham, Workshop Material from Session 12, Chemical Engineering Summer School, Snowbird, Utah, Aug., 1997.

# Matlab Solutions To The Chemical Engineering Problem Set

**Chyi-Tsong Chen**



## Matlab Solutions To The Chemical Engineering Problem Set:

**Numerical Methods with Chemical Engineering Applications** Kevin D. Dorfman, Prodromos Daoutidis, 2017-01-11  
Designed primarily for undergraduates but also graduates and practitioners this textbook integrates numerical methods and programming with applications from chemical engineering Combining mathematical rigor with an informal writing style it thoroughly introduces the theory underlying numerical methods its translation into MATLAB programs and its use for solving realistic problems Specific topics covered include accuracy convergence and numerical stability as well as stiffness and ill conditioning MATLAB codes are developed from scratch and their implementation is explained in detail all while assuming limited programming knowledge All scripts employed are downloadable and built in MATLAB functions are discussed and contextualised Numerous examples and homework problems from simple questions to extended case studies accompany the text allowing students to develop a deep appreciation for the range of real chemical engineering problems that can be solved using numerical methods This is the ideal resource for a single semester course on numerical methods as well as other chemical engineering courses taught over multiple semesters *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 algebraic 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](http://www.cambridge.org/9780521859714) *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

*Problem Solving in Chemical and Biochemical Engineering with POLYMATH, Excel, and MATLAB* Michael B. Cutlip, Mordechai Shacham, 2008 Problem Solving in Chemical and Biochemical Engineering with POLYMATH Excel and MATLAB Second Edition is a valuable resource and companion that integrates the use of numerical problem solving in the three most widely used software packages POLYMATH Microsoft Excel and MATLAB Recently developed POLYMATH capabilities allow the automatic creation of Excel spreadsheets and the generation of MATLAB code for problem solutions Students and professional engineers will appreciate the ease with which problems can be entered into POLYMATH and then solved independently in all three software packages while taking full advantage of the unique capabilities within each package The book includes more than 170 problems requiring numerical solutions This greatly expanded and revised second edition includes new chapters on getting started with and using Excel and MATLAB It also places special emphasis on biochemical engineering with a major chapter on the subject and with the integration of biochemical problems throughout the book

General Topics and Subject Areas Organized by Chapter Introduction to Problem Solving with Mathematical Software Packages Basic Principles and Calculations Regression and Correlation of Data Introduction to Problem Solving with Excel Introduction to Problem Solving with MATLAB Advanced Problem Solving Techniques Thermodynamics Fluid Mechanics Heat Transfer Mass Transfer Chemical Reaction Engineering Phase Equilibrium and Distillation Process Dynamics and Control Biochemical Engineering Practical Aspects of Problem Solving Capabilities Simultaneous Linear Equations Simultaneous Nonlinear Equations Linear Multiple Linear and Nonlinear Regressions with Statistical Analyses Partial Differential Equations Using the Numerical Method of Lines Curve Fitting by Polynomials with Statistical Analysis Simultaneous Ordinary Differential Equations Including Problems Involving Stiff Systems Differential Algebraic Equations and Parameter Estimation in Systems of Ordinary Differential Equations The Book's Web Site <http://www.problemsolvingbook.com> Provides solved and partially solved problem files for all three software packages plus additional materials Describes discounted purchase options for educational version of POLYMATH available to book purchasers Includes detailed selected problem solutions in Maple Mathcad and Mathematica

**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 BOOK JACKET Title Summary field provided by Blackwell North America Inc All Rights Reserved

**Applied Mathematical Methods for Chemical Engineers** Norman W. Loney, 2016-03-09 This book uses worked examples to showcase several mathematical methods that are essential to solving real world process engineering problems The third edition includes additional examples related to process control Bessel Functions and contemporary areas such as drug delivery The author inserts more depth on specific applications such as nonhomogeneous cases of separation of variables adds a section on special types of matrices such as upper and lower triangular matrices incorporates examples related to biomedical engineering applications and expands the problem sets of numerous chapters

**Introduction to Chemical Engineering Computing** Bruce A. Finlayson, 2014-03-05 Step by step instructions enable chemical engineers to master key software programs and solve complex problems Today both students and professionals in chemical engineering must solve increasingly complex problems dealing with refineries fuel cells microreactors and pharmaceutical plants to name a few With this book as their guide readers learn to solve these problems using their computers and Excel MATLAB Aspen Plus and COMSOL Multiphysics Moreover they learn how to check their solutions and validate their results to make sure they have solved the problems correctly Now in its Second Edition Introduction to Chemical Engineering Computing is based on the author's firsthand teaching experience As a result the emphasis is on problem solving Simple introductions help readers become conversant with each program and then tackle a broad range of problems in chemical engineering including Equations of state Chemical reaction equilibria Mass balances with recycle streams Thermodynamics and simulation of mass transfer equipment Process simulation Fluid flow in two and three dimensions All the chapters contain clear instructions figures and examples to guide readers through all the programs and types of chemical engineering problems Problems at the end of each chapter ranging from simple to difficult allow readers to gradually build their skills whether they solve the problems themselves or in teams In addition the book's accompanying website lists the core principles learned from each problem both from a chemical engineering and a computational perspective Covering a broad range of disciplines and problems within chemical

engineering Introduction to Chemical Engineering Computing is recommended for both undergraduate and graduate students as well as practicing engineers who want to know how to choose the right computer software program and tackle almost any chemical engineering problem *Solving Problems in Scientific Computing Using Maple and MATLAB®* Walter Gander, Jiri Hrebicek, 2004-06-07 Teaches problem solving using two of the most important mathematical software packages Maple and MATLAB This new edition contains five completely new chapters covering new developments Proceedings of Sixth International Conference on Soft Computing for Problem Solving Kusum Deep, Jagdish Chand Bansal, Kedar Nath Das, Arvind Kumar Lal, Harish Garg, Atulya K. Nagar, Millie Pant, 2017-02-22 This two volume book gathers the proceedings of the Sixth International Conference on Soft Computing for Problem Solving SocProS 2016 offering a collection of research papers presented during the conference at Thapar University Patiala India Providing a veritable treasure trove for scientists and researchers working in the field of soft computing it highlights the latest developments in the broad area of Computational Intelligence and explores both theoretical and practical aspects using fuzzy logic artificial neural networks evolutionary algorithms swarm intelligence soft computing computational intelligence etc 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 *Chemical Engineering Progress*, 2008 *Chemical Engineering Education*, 2004 **Innovations in Engineering Education**, 2005 Basic Principles and Calculations in Chemical Engineering David M. Himmelblau, James B. Riggs, 2012-05-31 The Number One Guide to Chemical Engineering Principles Techniques Calculations and Applications Now Even More Current Efficient and Practical Basic

Principles and Calculations in Chemical Engineering Eighth Edition goes far beyond traditional introductory chemical engineering topics presenting applications that reflect the full scope of contemporary chemical petroleum and environmental engineering Celebrating its fiftieth Anniversary as the field s leading practical introduction it has been extensively updated and reorganized to cover today s principles and calculations more efficiently and to present far more coverage of bioengineering nanoengineering and green engineering Offering a strong foundation of skills and knowledge for successful study and practice it guides students through formulating and solving material and energy balance problems as well as describing gases liquids and vapors Throughout the authors introduce efficient consistent student friendly methods for solving problems analyzing data and gaining a conceptual application based understanding of modern chemical engineering processes This edition s improvements include many new problems examples and homework assignments Coverage includes Modular chapters designed to support introductory chemical engineering courses of any length Thorough introductions to unit conversions basis selection and process measurements Consistent sound strategies for solving material and energy balance problems Clear introductions to key concepts ranging from stoichiometry to enthalpy Behavior of gases liquids and solids ideal real gases single component two phase systems gas liquid systems and more Self assessment questions to help readers identify areas they don t fully understand Thought discussion and homework problems in every chapter New biotech and bioengineering problems throughout New examples and homework on nanotechnology environmental engineering and green engineering Extensive tables charts and glossaries in each chapte Many new student projects Reference appendices presenting atomic weights and numbers Pitzer Z factors heats of formation and combustion and more Practical readable and exceptionally easy to use Basic Principles and Calculations in Chemical Engineering Eighth Edition is the definitive chemical engineering introduction for students license candidates practicing engineers and scientists This is the digital version of the print title Access to the CD content that accompanies the print title is available through product registration See the instructions in back pages of your digital edition CD ROM INCLUDES The latest Polymath trial software for solving linear nonlinear and differential equations and regression problems Point and click physical property database containing 700 compounds Supplemental Problems Workbook containing 100 solved problems Descriptions and animations of modern process equipment Chapters on degrees of freedom process simulation and unsteady state material balances Expert advice for beginners on problem solving in chemical engineering [Applied Numerical Methods with MATLAB for Engineers and Scientists](#) Steven C. Chapra,2008 Still brief but with the chapters that you wanted Steven Chapra s new second edition is written for engineering and science students who need to learn numerical problem solving This text focuses on problem solving applications rather than theory using MATLAB throughout Theory is introduced to inform key concepts which are framed in applications and demonstrated using MATLAB The new second edition feature new chapters on Numerical Differentiation Optimization and Boundary Value Problems ODEs **Handbook of Chemical Reactor Design,**

**Optimization, and Scaleup** Bruce Nauman, 2001-10-21 THE MODERN GUIDE TO CHEMICAL REACTORS In the best professional sourcebook on chemical reactors ever written world class expert Bruce Nauman provides too information and hands on expertise to make important engineering tasks and decisions easier Clearly and in depth CHEMICAL REACTOR DESIGN OPTIMIZATION AND SCALEUP provides Up to date information to help chemical and process engineers save time money and materials Decision aiding coverage of every aspect of selection design factors and parameters optimization and scaleup A convenient source of explained formulas principles and data Numerous detailed examples Worked mathematical solutions The latest information on reactor design for biochemicals and polymers as well as other newer and standard substances DESIGN AND SPECIFY CHEMICAL REACTORS CONFIDENTLY WITH STATE OF THE ART SKILLS

Numerical Techniques for Chemical and Biological Engineers Using MATLAB® Said S.E.H. Elnashaie, Frank Uhlig, Chadia Affane, 2007 This book addresses the bifurcation characteristics of chemical and biological processes as the general case and treats systems with a unique steady as special cases Back cover *Advanced Research on Industry, Information System and Material Engineering, IISME2011*

Helen Zhang, Gang Shen, David Jin, 2011-02-21 Selected peer reviewed papers from the 2011 International Conference on Industry Information System and Material Engineering IISME 2011 April 16 17 2011 Guangzhou China 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 MATLAB 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

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**Introductory Chemical Engineering Thermodynamics** J. Richard Elliott, Carl T. Lira, 2012-02-06 A  
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