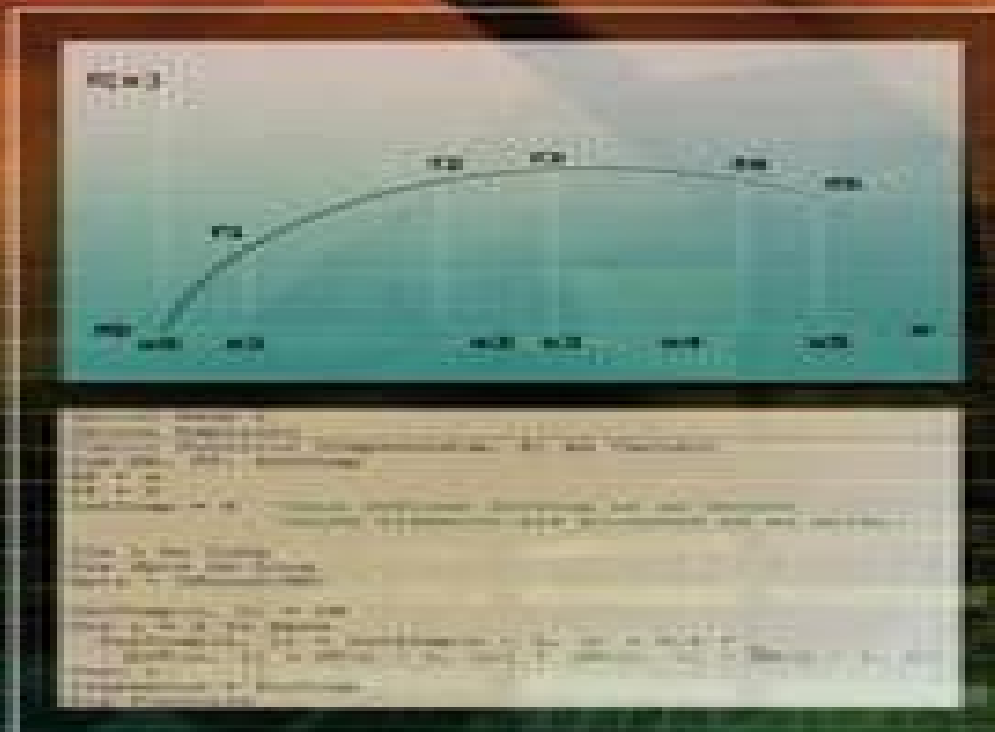


# NUMERICAL METHODS for CHEMICAL ENGINEERS Using Excel, VBA, and MATLAB



**VICTOR J. LAW**



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# Numerical Methods For Chemical Engineers Using Excel Vba And Matlab

**Navid Mostoufi,Alkis Constantinides**

## **Numerical Methods For Chemical Engineers Using Excel Vba And Matlab:**

Numerical Methods for Chemical Engineers Using Excel, VBA, and MATLAB Victor J. 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 **Introduction to Modeling and Numerical Methods for Biomedical and Chemical Engineers** Edward Gatzke, 2021-09-02 This textbook introduces the concepts and tools that biomedical and chemical engineering students need to know in order to translate engineering problems into a numerical representation using scientific fundamentals Modeling concepts focus on problems that are directly related to biomedical and chemical engineering A variety of computational tools are presented including MATLAB Excel Mathcad and COMSOL and a brief introduction to each tool is accompanied by multiple computer lab experiences The numerical methods covered are basic linear algebra and basic statistics and traditional methods like Newton s method Euler Integration and trapezoidal integration The book presents the reader with numerous examples and worked problems and practice problems are included at the end of each chapter Chemical Engineering Analysis and Optimization Using MATLAB Weiguo Xie, Sam Toan, Richard Davis, 2025-01-22 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 **Chemometrics** Richard G. Brereton, 2018-05-29 A new full color completely updated edition of the key practical guide to chemometrics This new edition of this practical guide on chemometrics emphasizes the principles and applications behind the main ideas in the field using numerical and graphical examples which can then be applied to a wide variety of problems in chemistry biology chemical engineering and allied disciplines Presented in full color it features expansion of the principal component analysis

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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 *Practical Numerical Methods for*

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*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

**Practical Numerical Methods for**

**Chemical Engineers** Richard A. Davis, 2014-09-24 This latest 3rd edition expands the breadth of Practical Numerical Methods with over 100 VBA macros for extending Excel's power for engineering and scientific analysis. Engineers and scientists will find the enhanced coverage of computational tools applicable to a variety of problems in their own disciplines. The selection of software reflects Excel's status as the de facto computational tool used by practicing engineers. Engineers/scientists should become proficient at extending Excel's capabilities with VBA programming to boost their worksheets with time-saving enhancements and powerful numerical techniques. Topics include an introduction to modeling documentation, Excel VBA root finding for linear/nonlinear systems of equations, multivariate optimization, experimental uncertainty propagation analysis, least squares regression, model validation, interpolation, integration, and ordinary/partial differential equations. A companion web site has links to digital files for downloading up to 200 illustrations, examples, the refined PNM3Suite workbook with VBA user-defined functions, macros, user forms for advanced numerical techniques. Practice problems are also available from the web site <https://www.d.umn.edu/~rdavis/PNM/PNMExcelVBA3>. Example files/macros are ready to be modified by users for their own needs. Chapter 1 includes a brief introduction to chemical reaction engineering that provides some background needed for problems involving mass/energy balances with reactions. The next two chapters introduce frequently overlooked features of Excel and VBA for engineering programming to apply numerical methods in Excel as well as document results. The remaining chapters present powerful numerical techniques using Excel VBA, including: General Methods, Sub/User-defined Function Procedures, Pseudo-random Number Generation, Sorting, Formula Graphing, Evaluation, Random Sampling, User forms, Linear Equations, Gaussian Elimination with Maximum Column Pivoting, Error Correction, Crout Reduction, Thomas algorithm for tri-diagonal, Cholesky's method for symmetric matrices, Matrix functions, Jacobi, Gauss-Seidel, Iteration, Wegstein, Steffenson's version of Aitkin's Delta-Square methods, Power method for Eigenproblems, Nonlinear Equations, Ordinary Fixed Point Iteration, Bisection, Secant, Regula Falsi, Newton, Quasi-Newton, Continuation, homotopy, Goal Seek Solver, Bairstow's method for polynomial roots, Derivative Approximation, Finite Difference, Richardson's extrapolation, Jacobian, Sensitivity Analysis, Lagrange polynomials, splines, Uncertainty Analysis, Jitter method for the Law of Propagation of Uncertainty, Monte Carlo with Latin Hypercube sampling, Jack-knife for regression parameter uncertainty, Optimization, Graphical Quadratic with acceleration, Powell, Golden Section, Luus-Jaakola Solver for linear and nonlinear programming, Parameter Scaling, Least squares Regression, multivariate linear models, Gauss-Newton, Levenberg-Marquardt, and Monte Carlo for nonlinear regression with parameter uncertainty, Rational Least Squares, Weighting, Interpolation, Linear-Newton, Divided Difference, Lagrange, Rational, Stineman, Cubic Spline, Constrained Splines, Bivariate 2-D Data Smoothing, Integration, Trapezoid, Improper Midpoint, Romberg, Adaptive Gauss-Kronrod, Simpson, Splines, multiple integrals with Simpson, Kronrod, Monte Carlo methods, Initial Value ODEs, Taylor Series, improved/modified Euler, implicit Trapezoidal for stiff problems, fixed variable, single step, 4-5 order Runge-Kutta, Cash-Karp, Dormand-Prince, Adams-Bashforth.

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**Catalog** University of Colorado Boulder, 2006

**Numerical Methods and Modeling for Chemical Engineers** Mark E. Davis, 2013-01-01 Geared toward advanced undergraduates or graduate students of chemical engineering studying applied mathematics this text introduces the quantitative treatment of differential equations arising from modeling physical phenomena in chemical engineering Coverage includes topics such as ODE IVPs placing emphasis on numerical methods and modeling implemented in commercial mathematical software available in 1985

**Numerical Methods for Engineers** Steven C. Chapra, Raymond P. Canale, 2002 The Fourth Edition of Numerical Methods for Engineers continues the tradition of excellence it established as the winner of the ASEE Meriam Wiley award for Best Textbook Instructors love it because it is a comprehensive text that is easy to teach from Students love it because it is written for them with great pedagogy and clear explanations and examples throughout This edition features an even broader array of applications including all engineering disciplines The revision retains the successful pedagogy of the prior editions Chapra and Canale's unique approach opens each part of the text with sections called Motivation Mathematical Background and Orientation preparing the student for what is to come in a motivating and engaging manner Each part closes with an Epilogue containing sections called Trade Offs Important Relationships and Formulas and Advanced Methods and Additional References Much more than a summary the Epilogue deepens understanding of what has been learned and provides a peek into more advanced methods What's new in this edition A shift in orientation toward more use of software packages specifically MATLAB and Excel with VBA This includes material on developing MATLAB m files and VBA macros In addition the text has been updated to reflect improvements in MATLAB and Excel since the last edition Also many more and more challenging problems are included The expanded breadth of engineering disciplines covered is especially evident in the problems which now cover such areas as biotechnology and

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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

**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

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**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 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) 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

**An Introduction to Numerical Methods for Chemical Engineers** James B. Riggs, 1988 In this second edition the author has added new problems and updated the accompanying FORTRAN computer programs New library programs are included that perform singular value decomposition of a matrix and apply a conjugate gradient optimizer Discussions have been added on the effect of stiffness on initial value problems and order variable step size integration An IBM compatible disk is included and an Apple and Macintosh disk as well as a solutions manual are available on request Annotation copyright by Book News Inc Portland OR

**Applied Mathematics and Modeling for Chemical Engineers** Richard G. Rice, Duong D. Do, James E. Maneval, 2023-03-07 Understand the fundamentals of applied mathematics with this up to date introduction Applied mathematics is the use of mathematical concepts and methods in various applied or practical areas including engineering computer science and more As engineering science expands the ability to work from mathematical principles to solve and understand equations has become an ever more critical component of engineering fields New engineering processes and materials place ever increasing mathematical demands on new generations of engineers who are looking more and more to applied mathematics for an expanded toolkit Applied Mathematics and Modeling for Chemical Engineers provides this toolkit in a comprehensive and easy to understand introduction Combining classical analysis of modern mathematics with more modern applications it offers everything required to assess and solve mathematical problems in chemical engineering Now updated to reflect contemporary best practices and novel applications this guide promises to situate readers in a 21st century chemical engineering field in which direct knowledge of mathematics is essential Readers of the third edition of Applied Mathematics and Modeling for Chemical Engineers will also find Detailed treatment of ordinary differential equations ODEs and partial differential equations PDEs and their solutions New material concerning approximate solution

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**Numerical Methods with Worked Examples: Matlab Edition** C. Woodford, C. Phillips, 2011-09-08 This book is for students following an introductory course in numerical methods numerical techniques or numerical analysis It introduces MATLAB as a computing environment for experimenting with numerical methods It approaches the subject from a pragmatic viewpoint theory is kept at a minimum commensurate with comprehensive coverage of the subject and it contains abundant worked examples which provide easy understanding through a clear and concise theoretical treatment This edition places even greater emphasis on learning by doing than the previous edition Fully documented MATLAB code for the numerical methods described in the book will be available as supplementary material to the book on <http://extras.springer.com>

*Applied Mathematical Methods for Chemical Engineers, Second Edition* Norman W. Loney, 2006-09-22 Focusing on the application of mathematics to chemical engineering Applied Mathematical Methods for Chemical Engineers Second Edition addresses the setup and verification of mathematical models using experimental or other independently derived data An expanded and updated version of its well respected predecessor this book uses worked examples to illustrate several mathematical methods that are essential in successfully solving process engineering problems The book first provides an introduction to differential equations that are common to chemical engineering followed by examples of first order and linear second order ordinary differential equations ODEs Later chapters examine Sturm Liouville problems Fourier series integrals linear partial differential equations PDEs and regular perturbation The author also focuses on examples of PDE applications as they relate to the various conservation laws practiced in chemical engineering The book concludes with discussions of dimensional analysis and the scaling of boundary value problems and presents selected numerical methods and available software packages New to the Second Edition Two popular approaches to model development shell balance and conservation law balance One dimensional rod model and a planar model of heat conduction in one direction Systems of first order ODEs Numerical method of lines using MATLAB and Mathematica where appropriate This invaluable resource provides a crucial introduction to mathematical methods for engineering and helps in choosing a suitable software package for computer based algebraic applications

*Numerical Methods with Worked Examples* Chris Woodford, C. Woodford, Chris Phillips, 1997-08-31 This book is for students following a module in numerical methods numerical techniques or numerical analysis It approaches the subject from a pragmatic viewpoint appropriate for the modern student The theory is kept to a minimum commensurate with comprehensive coverage of the subject and it contains abundant worked examples which provide easy understanding through a clear and concise theoretical treatment

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