INTRODUCTION TO
NUMERICAL METHODS IN CHEMICAL ENGINEERING

$$\frac{dC_j}{dx} = 0, j = A, B, C, D$$
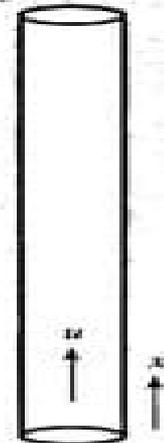
$$A + B \xrightarrow{k_1} C$$
$$B + C \xrightarrow{k_2} D$$

$$D\frac{d^2C_A}{dx^2} - u\frac{dC_A}{dx} - k_1 C_A C_B = 0$$

$$D\frac{d^2C_B}{dx^2} - u\frac{dC_B}{dx} - k_1 C_A C_B - k_2 C_B C_C = 0$$

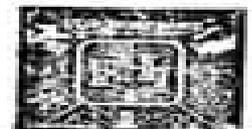$$D\frac{d^2C_C}{dx^2} - u\frac{dC_C}{dx} + k_1 C_A C_B - k_2 C_B C_C = 0$$

$$D\frac{d^2C_D}{dx^2} - u\frac{dC_D}{dx} + k_2 C_B C_C = 0$$

$$D\frac{d^2C_i}{dx^2} = D\frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2}$$

$$u\frac{dC_i}{dx} = u\frac{C_i - C_{i-1}}{\Delta x}$$

$$u C_{jin} = u C_j - D\frac{dC_j}{dx}$$

PHI

Pradeep Ahuja

Introduction To Numerical Methods In Chemical Engineering

AHUJA, PRADEEP

Introduction To Numerical Methods In Chemical Engineering:

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   **An Introduction to Numerical Methods for Chemical Engineers** James B. Riggs,1994 In this second edition of An Introduction to Numerical Methods for Chemical Engineers the author has revised text added new problems and updated the accompanying computer programs The result is a text that puts students on the cutting edge of solving relevant chemical engineering problems Designed explicitly for undergraduates this book provides students with software and experience to solve a number of problems Included in the text are Numerical algorithms in explicit detail Example problems from thermodynamic fluid flow heat transfer mass transfer kinetics and process design Equations developed specifically for the student from the example problems An introduction to advanced numerical techniques such as finite elements singular value decomposition and arc length homotopy An introduction to optimization A systematic approach to process modeling presented with advanced modeling examples The software that accompanies the book is for IBM compatible PCs A solution manual is also available upon request An Introduction to Numerical Methods for Chemical Engineers was first published in 1988 and has been taught in universities throughout the nation   An Introduction to Numerical Methods for Chemical Engineers (2nd Ed.) James B. Riggs,1994-01-15   An introduction to numerical methods for chemical engineers James B. Riggs,1988   **Numerical Methods and Modeling for Chemical Engineers** Mark E. Davis,2013-11-19 This text introduces the quantitative treatment of differential equations arising from modeling physical phenomena in chemical engineering Coverage includes

recent topics such as ODE IVPs emphasizing numerical methods and modeling of 1984 era commercial mathematical software **A Numerical Primer for the Chemical Engineer** Edwin Zondervan,2014-08-12 Solve Developed Models in a Numerical FashionDesigned as an introduction to numerical methods for students A Numerical Primer for the Chemical Engineer explores the role of models in chemical engineering Combining mathematical correctness model verification with numerical performance model validation this text concentrates on numerical metho **INTRODUCTION TO NUMERICAL METHODS IN CHEMICAL ENGINEERING.** PRADEEP. AHUJA,2019 **A Numerical Primer for the Chemical Engineer, Second Edition** Edwin Zondervan,2019-08-16 Designed as an introduction to numerical methods for students this book combines mathematical correctness with numerical performance and concentrates on numerical methods and problem solving It applies actual numerical solution strategies to formulated process models to help identify and solve chemical engineering problems Second edition comes with additional chapter on numerical integration and section on boundary value problems in the relevant chapter Additional material on general modelling principles mass energy balances and separate section on DAE s is also included Case study section has been extended with additional examples

Introduction to Numerical Methods with Application to Chemical Engineering Emad Ali,Abdelhamid Ajbar,Khalid Alhumaizi,2009 Many chemical engineering departments in diverse universities around the world including the one in King Saud University include in the curriculum a course designed to teach numerical methods applied to chemical engineering This book is essentially a compilation of the notes the three authors have used to teach this course over the years We have covered in the textbook the numerical techniques that are most useful to the chemical engineer and that have wide applications As an introduction to the book we included a chapter dealing with some practical considerations in numerical methods The concepts of errors conditioning of a problem and stability of algorithms were introduced to show the student to what extent he should trust any numerical values obtained by solving a problem in a digital computer tt from Preface p v

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   *Numerical Methods for Chemical Engineering* Kenneth J. Beers,2007 Applications of numerical mathematics and scientific computing to chemical engineering   **Computational Engineering - Introduction to Numerical Methods** Michael Schäfer,2006-05-01 This book is an introduction to modern numerical methods in engineering It covers applications in fluid mechanics structural mechanics and heat transfer as the most relevant fields for engineering disciplines such as computational engineering scientific computing mechanical engineering as well as chemical and civil engineering The content covers all aspects in the interdisciplinary field which are essential for an up to date engineer   **A Practical Introduction to Numerical Methods for Materials Scientists and Engineers** David Keffer,2015-09-21 This book presents an introduction to numerical methods targeted at undergraduate materials scientists and engineers What we hope to achieve through this text is a situation where the model formulation proceeds without regard for the ease of numerical solution Once the model is rigorously formulated the appropriate numerical solution is then identified Thus the science guides the numerical techniques rather than the other way around The philosophy espoused in this book is to equip the student with a compact but broadly applicable set of practical problem solving tools such that the student emerges at the end of the course with the belief If I can formulate the problem as a mathematical model I can solve it   **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   Numerical Methods in Chemical Engineering Using Python® and Simulink® Nayef Ghasem,2023-07-17 Numerical methods are vital to the practice of chemical engineering allowing for the solution of real world problems Written in a concise and practical format this textbook introduces readers to the numerical methods required in the discipline of chemical engineering and enables them to validate their solutions using both Python and Simulink Introduces numerical methods followed by the solution of linear and nonlinear algebraic equations Deals with the numerical integration of a definite function and solves initial and boundary value ordinary differential equations with different orders Weaves in examples of various numerical methods and validates solutions to each with Python and Simulink graphical programming Features appendices on how to use Python and Simulink Aimed at advanced undergraduate and graduate chemical engineering students as well as practicing chemical engineers this textbook offers a guide to the use of two of the most widely used programs in the discipline The textbook features numerous video lectures of applications and a solutions manual for qualifying instructors   **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 **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 **Computational Methods in Chemical Engineering** Owen T. Hanna,Orville C. Sandall,1995 Authors Owen Hanna and Orville Sandall include broad use of convergence acceleration techniques such as Pade approximation for series Shanks transformation for series linear and nonlinear systems of algebraic equations systematic use of global Richardson extrapolation for integrals and ODE systems to monitor the overall error and discussion of methods for the solution of stiff ODE **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

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