

# INTRODUCTION TO NUMERICAL METHODS IN CHEMICAL ENGINEERING

$$\frac{dC_j}{dx} = 0, j = A, B, C, D$$



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

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

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

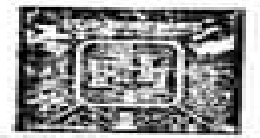
$$D \frac{d^2 C_D}{dx^2} - u \frac{dC_D}{dx} + k_2 C_B C_C = 0$$



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

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

$$u C_{i+1} = u C_i - D \frac{dC_i}{dx}$$



# Introduction To Numerical Methods In Chemical Engineering

**CO Houle**



## **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 the 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** James B. Riggs, 1988 *An Introduction to Numerical Methods for Chemical Engineers (2nd Ed.)* James B. Riggs, 1994-01-15 A *Numerical Primer for the Chemical Engineer* Edwin Zondervan, 2014-08-12 Solve Developed Models in a Numerical Fashion. Designed 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

*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

[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

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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

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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 *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 **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

*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**

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