

# Lecture #01

## Finite Difference-based Numerical Methods in Chemical Engineering

### Recommended Books:

- 1) Numerical Methods for Engineers (Gupta)
- 2) Numerical Methods for Engineering Application (Ferziger)
- 3) Linear Algebra (Strang)

**Objective:** Learn a few basic numerical techniques (Finite Difference) to solve simple ODEs/PDEs/algebraic equations derived from a variety of heat and mass transfer related conservation equations.

- Analytical methods yield exact solutions, often in infinite series, use mathematical functions.
- Numerical methods yield approximate solutions, use numbers, computations, results are dependent on the method accuracies and limited by computers machine errors.

*Course focuses on*

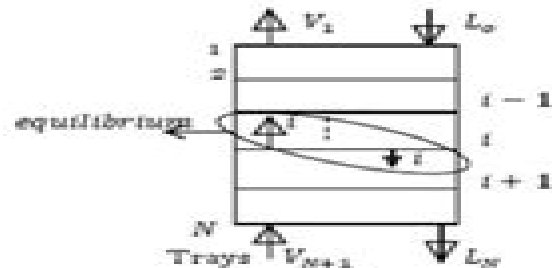
- Algebra (Matrix Operation)
- Methods (Finite Difference)

*Requires knowledge of*

- Computer Programming (because large # of iterations)  
(there are engineering software, e.g., Matlab, NAG, IMSL, Polymath)
- No numerical analysis in this course!

**Examples:** (Applications in chemical engineering)

### 1. Distillation



**Assume:** Constant molar flowrates of vapor & liquid

Binary components:  $A$ ,  $B$

(more volatile)

Species balance on  $i^{th}$  plate:

# Numerical Methods In Chemistry

**James B. Riggs**



## **Numerical Methods In Chemistry:**

*Maths in Chemistry* Prerna Bansal, 2020-09-07 Numerical methods are the mathematical procedures that approximate the solution of complex mathematical problems into much simpler form and which find a wide variety of use while solving complex Physical Chemistry problems This book aims to aide in understanding of such numerical methods including solving complex differential equations and numerical differentiation integration Moreover it also explains various statistical tests used in Analytical Chemistry for data analysis The author has tried to include as many example from Chemistry problems for a better understanding of the methods

**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 Chemistry A. C. Norris, 1981 **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

*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

Computational Chemistry Anthony Charles Norris, 1981 *Numerical Methods in Chemistry* Kenneth Jeffrey Johnson, 1972 **Tensor Numerical Methods in Quantum Chemistry** Venera Khoromskaia, Boris N. Khoromskij, 2018-06-11 The conventional numerical methods when applied to multidimensional problems suffer from the so called curse of dimensionality that cannot be eliminated by using parallel architectures and high performance computing The novel tensor numerical methods are based on a smart rank structured tensor representation of the multivariate functions and operators discretized on Cartesian grids thus reducing solution of the multidimensional integral differential equations to 1D calculations We explain basic tensor formats and algorithms and show how the orthogonal Tucker tensor decomposition originating from chemometrics made a revolution in numerical analysis relying on rigorous results from approximation theory Benefits of tensor approach are demonstrated in ab initio electronic structure calculations Computation of the 3D convolution integrals for functions with multiple singularities is replaced by a sequence of 1D operations thus enabling accurate MATLAB calculations on a laptop using 3D uniform tensor grids of the size up to  $10^{15}$  Fast tensor based Hartree Fock solver incorporating the grid based low rank factorization of the two electron integrals serves as a prerequisite for economical calculation of the excitation energies of molecules Tensor approach suggests efficient grid based numerical treatment of the long range electrostatic potentials on large 3D finite lattices with defects The novel range separated tensor

format applies to interaction potentials of multi particle systems of general type opening the new prospects for tensor methods in scientific computing This research monograph presenting the modern tensor techniques applied to problems in quantum chemistry may be interesting for a wide audience of students and scientists working in computational chemistry material science and scientific computing **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 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

**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 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 are 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.

**Chemical Modelling** Alan Hinchliffe, 2007-10-31. Chemical Modelling: Applications and Theory comprises critical literature reviews of molecular modelling, both theoretical and applied. Molecular modelling in this context refers to modelling the structure, properties, and reactions of atoms, molecules, materials. Each chapter is compiled by experts in their fields and provides a selective review of recent literature. With chemical modelling covering such a wide range of subjects, this Specialist Periodical Report serves as the first port of call to any chemist, biochemist, materials scientist, or molecular physicist needing to acquaint themselves of major developments in the area. Specialist Periodical Reports provide systematic and detailed review coverage in major areas of chemical research. Compiled by teams of leading authorities in the relevant subject areas, the series creates a unique service for the active research chemist with regular, in-depth accounts of progress in particular fields of chemistry. Subject coverage within different volumes of a given title is similar, and publication is on an annual or biennial basis. Current subject areas covered are: Amino Acids, Peptides, and Proteins; Carbohydrate Chemistry; Catalysis; Chemical Modelling: Applications and Theory; Electron Paramagnetic Resonance; Nuclear Magnetic Resonance; Organometallic Chemistry; Organophosphorus Chemistry; Photochemistry; and Spectroscopic Properties of Inorganic and Organometallic Compounds. From time to time, the series has altered according to the fluctuating degrees of activity in the various fields, but these volumes remain a superb reference point for researchers.

**Tensor Numerical Methods in Electronic Structure Calculations** Venera

Khoromskaia, Boris Khoromskij, 2016      *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  
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 integration An IBM compatible disk is included and an Apple and Macintosh disk as well as a solutions manual are available  
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 Michael B. Cutlip, Mordechai Shacham, 1999 A companion book including interactive software for students and professional  
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 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      **Practical Data Analysis in Chemistry** Marcel Maeder,Yorck-Michael Neuhold,2007-08-10 The majority of modern instruments are computerised and provide incredible amounts of data Methods that take advantage of the flood of data are now available importantly they do not emulate graph paper analyses on the computer Modern computational methods are able to give us insights into data but analysis or data fitting in chemistry requires the quantitative understanding of chemical processes The results of this analysis allows the modelling and prediction of processes under new conditions therefore saving on extensive experimentation Practical Data Analysis in Chemistry exemplifies every aspect of theory applicable to data analysis using a short program in a Matlab or Excel spreadsheet enabling the reader to study the programs play with them and observe what happens Suitable data are generated for each example in short routines this ensuring a clear understanding of the data structure Chapter 2 includes a brief introduction to matrix algebra and its implementation in Matlab and Excel while Chapter 3 covers the theory required for the modelling of chemical processes This is followed by an introduction to linear and non linear least squares fitting each demonstrated with typical applications Finally Chapter 5 comprises a collection of several methods for model free data analyses Includes a solid introduction to the simulation of equilibrium processes and the simulation of complex kinetic processes Provides examples of routines that are easily adapted to the processes investigated by the reader Model based analysis linear and non linear regression and model free analysis are covered



## Decoding **Numerical Methods In Chemistry**: Revealing the Captivating Potential of Verbal Expression

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