

## 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*

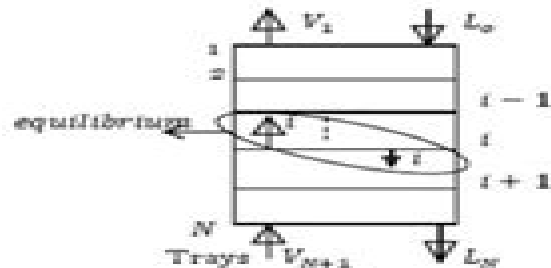
- Algebra (Matrix Operation)
- Methods (Finite Difference)

*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:  $A$ ,  $B$

$A$  (more volatile)

**Species balance on  $i^{\text{th}}$  plate:**

# Numerical Methods In Chemistry

**Kenneth Jeffrey Johnson**



## **Numerical Methods In Chemistry:**

*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

### **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

**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** Anthony Charles Norris, 1981      **Computational Chemistry** A. C. Norris, 1981      Maths in Chemistry Prerna Bansal, 2024-09-02

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 aid 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

**Numerical Methods in Chemistry** Kenneth Jeffrey Johnson, 1972      **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](http://www.cambridge.org) 9780521859714      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

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

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