

# SECOND SEMESTER 2023-2024

Course Handout Part II

Date: 21-12-2023

In addition to part-I (General Handout for all courses appended to the time table) this portion gives further specific details regarding the course.

*Course No.* : *ChE F242*

*Course Title* : Numerical Methods for Chemical Engineers

*Instructor-in-Charge* : Lakshminarayanan Samavedham

# Scope and Objective of the Course:

**Scope:**

This course provides students with key concepts of numerical methods and their applications to problems in thermodynamics, fluid mechanics, heat and mass transfer, and reaction engineering. The topics covered are solution of linear and nonlinear algebraic equation systems, multiple linear regression, interpolation, differentiation, integration, and solution of ordinary differential equations (initial and boundary value problems). Subject to availability of time, numerical solution of partial differential equations will also be covered. Each topic starts with an introduction of its applications in chemical engineering followed by principles and development of selected methods. Use of MATLAB for solution of the above model types will be demonstrated.

# Course Learning Outcomes:

Upon completing this course, the student must be able to:

1. Formulate mathematical and numerical models for typical chemical processes
2. Articulate the broad and specific principles employed in numerical algorithms
3. Demonstrate capability to use MATLAB and its toolboxes for implementing numerical algorithms and solving practical chemical engineering problems
4. Verify the correctness of the numerical solution and interpret the results

# Mode of Delivery:

This course will be conducted in the flipped class format. Course videos will be posted on the CMS and the videos to be completed each week will be spelt out in the course handout. The total duration of video time each week is about 165 minutes on average (less than 3 hours).

You are expected to watch the videos ahead of time before you come to class. If you have any doubts, drop by my office during the announced chamber consultation hours or via CMS/email and get the doubts sorted out.

The class will be randomly divided into 4 groups and each group will be assigned to one of the 4 time-tabled hours. Each student needs to show up in the classroom only during that particular hour. In that one hour, you will be given a few problems to solve individually and submit it to CMS in the first 25 minutes. Then, you will be

given a few problems to be solved in groups of 2 which you will complete and submit to CMS before you leave the class. These will be evaluated and be part of the grading process – each session will be worth 4% towards your final grade. There is no obligation for you to attend these sessions if you do not want the 4 marks.

# Textbooks:

1. Steven C. Chapra, Raymond P. Canale, “Numerical Methods for Engineers”, McGraw-Hill, 7th Edition, 2015, ISBN 978–0– 07–339792–4

# Reference books:

* 1. Stefan J. Chapman, “MATLAB Programming for Engineers”, Cengage Learning, 6th Edition, 2020 ISBN-10 : 935350287X, ISBN-13 : 978-9353502874

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**Software:** MATLAB

# Course Plan:

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| **Lecture No.** | **Learning objectives** | **Topics to be covered** | **Chapter & Section in Textbook** | **Videos from CMS** |
| 1 | Course Introduction and Overview | Course Introduction  Course Introduction (Roadmap) Course Introduction (Logistics and Operational Details) | Nil | 1 to 3 |
| 2-3 | Mathematical Models Overview and Classification | Introduction to Mathematical Models Classification of Models: Linear vs. Nonlinear Characteristics of Linear and Nonlinear Models  Classification of Models: Steady State vs. Dynamic  Classification of Models: Lumped vs. Distributed | Chapter 1  Section 1 | 4 to 8 |
| 4-6 | Construction of Mathematical Models | Where do Models come from? Mathematical Models for a Simple Reaction System and a Heated Plate  Mathematical Models Derived from First Principles  Dynamic Models of Typical Chemical Processes | Chapter 1  Section 2 | 9 to 18 |
| 7-9 | Technical Tour of Problem Types of Interest to Chemical Engineers | Linear and Nonlinear Algebraic Equation Systems and the use of algebraic mathematical models to solve an optimization problem will be introduced with Examples | Chapter 9  Chapter 12  Chapter 16 Section2 | 19 to 25 |
| 10-12 | Technical Tour of Problem Types of  Interest to Chemical Engineers | Ordinary Differential Equations (Initial and Boundary Value Problem), Functional  Approximation for Numerical Interpolation, Differentiation and Integration with Examples | Chapter 28  Sections 1  & 2 | 26 to 30 |
| 13 | Solution of Linear Equation Systems | Gauss Elimination | Chapter 9 | 31 to 32 |

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|  |  |  | Sections 1  to 4 |  |
| 14-15 | Solution of Linear Equation Systems (Contd.) | Concept of Pivoting in Solving Linear Equation Systems  Gauss Jordan Method and properties of residuals  The Concept of Ill-Conditioning Tridiagonal Equation Systems and the Thomas Algorithm  Introduction to Iterative Techniques to solve Linear Equation Systems | Chapter 9  Section 7  Chapter 9  Section 3  Chapter 7  Section 4 | 33 to 38.  (Video 37 has two parts 37A and 37B) |
| 16-18 | Iterative and Decomposition Methods for Solution of Linear Equation Systems | Concept of Diagonal Dominance  Jacobi and Gauss-Siedel Iterative Schemes The Concept of Spectral Radius Successive Over Relaxation with Gauss Siedel Method  Decomposition Methods | Chapter 10  Section 1  Chapter 11  Sections 1  & 2 | 39 to 43 |
| 18  (Contd.) | Introduction to Nonlinear Algebraic Equation Systems | Solving Nonlinear Equations Some Fundamentals | Chapter 6 | 44 |
| 19-22 | Numerical solution of nonlinear algebraic equation systems | Solving Single Nonlinear Equation with Newton Method  Newton Method for a System of Nonlinear Equations  Example of solving a single Nonlinear Equation  Examples of solving a System of Nonlinear Equations | Chapter 6  Section 2  Chapter 6  Section 6 | 45 to 49 |
| 22  (Contd.) | Multiple Linear Regression (MLR) | Introduction to Linear Regression | Chapter 17  Section 1 | 50 |
| 23-24 | Multiple Linear Regression (Contd.) | Linear Regression: Models convertible to linear form  The Mathematics behind Multiple Linear Regression  Fitting a Quadratic Trend  Introduction to Stepwise Tool in MATLAB Model for a Two-Input One-Output System Using Regression Model to Optimize Process  Settings | Chapter 17  Sections 2  to 4 | 51 to 56 |
| 25-26 | Functional Approximation | Introduction to Functional Approximation Some Basic Issues with Functional Approximation  Basis Functions for Functional Approximation  Functional Approximation with Cubic Splines | Chapter 18  Sections 1  & 6 | 57 to 60 |
| 27 | Numerical Interpolation | Interpolation with Lagrange Polynomials Introduction to Difference Operators | Chapter 18  Sections 2  & 3 | 61 to 62 |
| 28 | Numerical Interpolation | Newton Forward Difference Table and Polynomials | Chapter 18  Section 4 | 61 to 65 |

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|  |  | Inverse Interpolation |  |  |
| 29 | Numerical Differentiation | Numerical Differentiation First Derivative Numerical Differentiation Second Derivative | Chapter 23  Section 1 | 66 to 67 |
| 30 | Numerical Integration | Introduction to Numerical Integration Numerical Integration Trapezoid Rule Numerical Integration Simpsons Rules | Chapter 21  Sections 1  & 2 | 68 to 70 |
| 31 | Numerical Integration Advanced Topics | Numerical Integration Gauss Quadrature Improving Accuracy of Integral Estimates  Application of Romberg Extrapolation | Chapter 22  Sections 1,  2 & 4 | 71 to 73 |
| 32 | Ordinary Differential Equations (IVP) | Introduction to Ordinary Differential Equations and Initial Value Problems (IVPs) | Chapter 25 | 74 |
| 33 | Solution of Initial Value Problems | Solving IVPs using Euler Scheme Heun's Predictor-Corrector Method | Chapter 25 | 75 to 76 |
| 34-36 | Solution of Initial Value Problems | Solving IVPs using Euler Scheme Heun's Predictor-Corrector Method Runge-Kutta Methods  Overview of Runge-Kutta Explicit Method (RK4)  Illustration of RK4 Method with an Example Overview of Runge-Kutta Implicit Method (RK2)  Illustration of RK2 Method with an Example | Chapter 26 | 77 to 81 |
| 37 | Ordinary Differential Equations (BVP) | Introduction to Boundary Value Problems (BVPs) | Chapter 27 | 82 |
| 38-40 | Numerical Solution of Boundary Value Problems | Solving BVPs using Finite Difference Method BVP Example 1 using Finite Difference Method  BVP Example 2 using Finite Difference Method  BVP Example 3 using Finite Difference Method | Chapter 27 | 83 to 86 |

**Evaluation Scheme:**

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| **Component** | **Duration** | **Weightage (%)** | **Date & Time** | **Nature of Component** |
| Weekly Problem Solving Individual | 25  minutes | 24% | Once every week (12 weeks) during class hours | Open Book, Notes and using MATLAB |
| Weekly Problem Solving Group | 25  minutes | 24% | Once every week (12 weeks) during class hours | Open Book, Notes and using MATLAB |
| Midterm | 90  minutes | 20% | To be Announced | Open Book, Notes and using MATLAB |

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| Comprehensive | 3 Hours | 32% | 7 May 2023 AM | Open Book, Notes and using MATLAB |

**Chamber Consultation Hours:** 4-6 PM (Mondays, Wednesdays) at Block D, Room 319B. Students can contact me through CMS and I will try to respond as quickly as I can.

**Notices:** All notices and correspondences will be via the course management system (CMS). It is your responsibility to check the CMS and your BITS email for all information disseminated by me.

**Make-up Policy:** Make-up will be offered only for the mid-semester examination and will normally be held within one week of the mid-semester test. You need not give any proof to ask for the make-up. Only know that the make-up exam will be more difficult compared to the main test and the test format may also be different. If you are not able to take the make-up test on the day it is held, you will be awarded zero credit for the mid-semester test.

**Academic Honesty and Integrity Policy:** Students are professionals-in-training and are expected to be respectful and to each other and be fair to other learners. Any act of academic dishonestly will be dealt with as per the policies in place at BITS Pilani Hyderabad Campus.



Lakshminarayanan Samavedham

**INSTRUCTOR-IN-CHARGE**