Birla Institute of Technology & Science, Pilani
Hyderabad Campus

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, 7^{th} Edition, 2015, ISBN 978–0– 07–339792–4

Reference books:

1. Stefan J. Chapman, "MATLAB Programming for Engineers", Cengage Learning, 6^{th} Edition, 2020 ISBN-10 : 935350287X, ISBN-13 : 978-9353502874

.

Software: MATLAB

Course Plan:

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
			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

innovate achieve lead

28	Numerical Interpolation	Newton Forward Difference Table and Polynomials	Chapter 18 Section 4	61 to 65
		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:

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	20%	To be Announced	Open Book, Notes and

	minutes			using MATLAB
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