Birla Institute of Technology & Science, Pilani
Hyderabad Campus

SECOND SEMESTER 2024-2025
Course Handout (Part II)

Date: 06/01/2025

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: Dr. Arnab Dutta

1. Objective & Motivation:

The knowledge of numerical methods is essential to tackle real-life problems, which may not be possible to solve analytically. Numerical methods have always been a powerful tool to solve various complex physio-chemical phenomena spanning different domain. It is not only important to understand these algorithms but one also has to implement it with the help of computer codes. The amalgamation of these algorithms along with computer codes is necessary to get a complete flavor of this subject. In this course, you will be exposed to a variety of algorithms for solving algebraic and differential equations both from theoretical as well as computational perspective using MATLAB.

2. Learning Outcomes:

- Numerical techniques to solve linear and non-linear algebraic equations
- Solve ordinary and partial differential equations using numerical methods
- Numerical schemes to perform differentiation and integration
- Parameter estimation using regression techniques

3. Text Book:

Steven C. Chapra, Raymond P. Canale, "Numerical Methods for Engineers", Tata McGraw-Hill 6th Edition 2012.

4. Reference Books:

1. S. K. Gupta, "Numerical Methods for Engineers", New Age International Publishers 2nd Edition 2010.

2. Stefan J. Chapman "MATLAB Programming for Engineers", 4th Edition. Cengage Learning.

5. Course Plan:

Lec. No.	Learning Objectives	Topics to be covered	Resource*
1-2	Introduction	▪ Get to know the students ▪ Understand students' notion about the subject ▪ Introduction to the course ▪ Necessity of mathematical models & algorithms ▪ Computational tools for problem solving	--
2-3	Error analysis	▪ Significant digits ▪ Accuracy & precision ▪ Round off errors ▪ Truncation error ▪ Error propagation	Chapters: 3-4
4-9	Roots of Equations	▪ Bisection method ▪ False-position method ▪ Newton-Raphson's method ▪ Secant method ▪ Roots of polynomials	Chapters: 5-7
10-14	Linear Algebraic Equations	▪ Gauss elimination ▪ Gauss-Jordan ▪ LU decomposition ▪ Thomas algorithm ▪ Gauss-Seidel	Chapters: 9-11
15-18	Numerical Differentiation & Integration	▪ Differentiation technique ▪ Trapezoidal rule ▪ Simpson's rule	Chapters: 21-23
19-27	ODE-IVPs#	▪ Euler's method ▪ Adams-Bashforth & Adams-Moulton techniques ▪ Runge-Kutta methods ▪ Stiffness of ODEs ▪ Predictor-Corrector techniques ▪ Stability of algorithms	Chapters: 25-26
28-30	ODE-BVPs†	▪ Finite difference ▪ Shooting technique	Chapters: 27, 31
31-34	PDE ‡	▪ Elliptic equations ▪ Parabolic equations ▪ Finite difference	Chapters: 29-31
35-36	Curve Fitting	▪ Newton's divided difference interpolating polynomials ▪ Lagrangian interpolation	Chapter: 17-18
37-39	Optimization	▪ Introduction ▪ Problem formulation	Reference material will be provided
40	Course wrap-up		

* Unless otherwise specified all chapters are taken from the prescribed textbook.

Ordinary Differential Equations: Initial Value Problems

† Ordinary Differential Equations: Boundary Value Problems

‡ Partial Differential Equations

6. Evaluation Scheme:

Component	Duration (minutes)	Weightage (%)	Date & Time	Nature of Component
Mid-Term	90	25	03/03 2.00 - 03.30PM	Open Book
Assignments (2)	--	25	TBA in the class (Evenly distributed)	Open Book
Continuous Assessment	--	15	TBA in the class	Closed Book
Comprehensive Examination	180	35	02/05FN	Closed Book (15%) Open Book (20%)

7. **Tutorials:** Hand-on session using MATLAB. Please install MATLAB in your personal PCs.
8. **Consultation Hour:** Will be announced in the class. [Chamber: D216]
9. **Notices:** Notices concerning the course will be communicated via LMS.
10. **Make-up Policy:** Make-up is granted only for genuine cases with valid justifications at the discretion of the IC. A prior permission from the Instructor-in-charge is required. Decision of the IC will be final. There will be NO provision for Make-up w.r.t. assignments and continuous assessments.
11. **Academic Honesty and Integrity Policy:** Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

Arnab Dutta

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Instructor-in-charge
CHE F242