SECOND SEMESTER 2020-21
COURSE HANDOUT

Date: 18.01.2021

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	**:**	PRATIK N SHETH
Instructor(s)	**:**	Pratik N Sheth
Tutorial/Practical Instructors:		Ajay Kumar Pani and Ajita Neogi

1. Course Description:

Introduction to mathematical modeling and engineering problem solving, Use of software packages and programming, Errors and approximations including error propagation and numerical error, Roots of equations: Linear algebraic equations, 1-D and multi-dimensional unconstrained optimization including gradient methods, Linear programming, Non-linear constrained optimization, Optimization with packages, Least Squares Regression including quantification of error, Polynomial regression, Lagrange, inverse and spline interpolation and Fourier approximation, Engineering applications, Numerical differentiation and integration, Ordinary differential equations, Partial differential equations, Engineering applications.

2. Scope and Objective of the Course:

Several chemical engineering problems involve finding roots in a higher order equation, solving simultaneous set of algebraic equations, solving differential equations etc. Quite often, these equations are not amenable to analytical solutions. In such cases, use of numerical methods is necessary which then provides a way for the engineer to translate the language of mathematics and physics into information that may use to make engineering decisions. This course will provide students with an exposure to numerical techniques which can be used to solve algebraic and differential equations of varying complexity. Numerical methods for differentiation, integration and curve fitting techniques will also be covered. Strong emphasis will be placed on problem solving based on case studies in engineering. Specific focus in case studies will be application of numerical techniques and scientific computing to the practice of chemical engineering. The role of computers and software along with identification, quantification and minimization of errors involved in numerical analysis will also be highlighted.

3. Text Books:

Chapra, S. C. and R. P. Canale, Numerical Methods for Engineers, 7th Edition, McGraw Hill Education (India) Pvt. Ltd., New Delhi, 2015.

4. Reference Books:

Chapra, S. C., Applied Numerical Methods with MATLAB for Engineers and Scientists, 3rd Edition, McGraw Hill, 2012.

5. Course Plan:

Module No.	Lecture Session	Reference	Learning outcomes
1. Introduction, modeling, computer, error analysis	L1.1. Introduction to the course, significance in chemical engineering, Hand out discussion		To understand the fundamentals of problem formulation and differentiate between analytical and numerical solutions Importance of computers and the role of errors and approximations in the implementation of numerical methods
	L1.2. Concept of simple mathematical model, conservation laws and engineering, Role of programming and software, Introduction to MATLAB	**T: 1.1 – 1.2** **T: 2.1 – 2.5**	
	L1.3. Approximations and round off errors; Taylor series and truncation errors	**T: 3.1 – 3.4** **T: 4.1 – 4.4**	
2. Roots of equations	L2.1 Bracketing methods: Graphical, bisection and false position methods; Open Methods: Fixed point iteration method	**T: 5.1 – 5.4** **T: 6.1**	To apply the different numerical techniques for finding roots of equations, assess their reliability and choosing the best technique for a specific problem
	L2.2 Open Methods: Newton Raphson Secant and Brent's Methods	**T: 6.2 – 6.4**	
	L2.3 Multiple roots and system of nonlinear equations	**T: 6.5 – 6.6**	
	L2.4 Use of MATLAB to solve the various case studies	**T: 8.1 – 8.4**	
3. Linear Algebraic equations	L3.1 Linear algebraic equations and Engineering practice, Gauss Elimination, Naïve Gauss elimination	**T: 9.1 – 9.2**	To apply different techniques for Solving problems involving system of linear algebraic equations and assess their reliability and choosing the best technique for a particular problem
	3.2 pitfalls, Techniques for improving solutions, Gauss Jordan method	**T: 9.3, 9.4, 9.7**	
	3.3 LU Decomposition and Matrix Inversion methods	**T: 10.1 -10.3**	
	3.4 Special Matrices, Gauss Seidel method	**T:11.1 - 11.3**	
	3.5 Use of MATLAB to solve the various case studies	**T:12.1 - 12.4**	

4. Curve Fitting: regression and Interpolation	4.1 Linear Regression	**T:17.1**	Fitting curves (linear and non-linear) to experimental data and finding accuracy of a specific linear/non-linear model for a particular system
	4.2 Polynomial and multiple linear regression	**T:17.2 - 17.3**	
	4.3 General linear least squares and non linear regression	**T:17.4 - 17.5**	
	4.4 Newton's divided difference Interpolation, Lagrange's interpolation	**T:18.1 - 18.2**	
	4.5 Inverse interpolation, spline interpolation	**T:18.3 - 18.6**	
	4.6 Curve Fitting with software packages & Case studies	**T:19.8, 20.1 - 20.4**	
5. Numerical Differentiation and Integration	5.1 Trapezoidal rule, Simpson's 1/3 and 3/8 rule	**T:21.1 - 21.2**	To apply the numerical differentiation and integration techniques for engineering problem solving. Trade-offs involved in selecting the best method for a particular problem
	5.2 Unequal segment Integration	**T:21.3**	
	5.3 Differentiation formulas	**T:23.1 - 23.5**	
	5.4 Numerical differentiation and integration using MATLAB	**T:23.6**	
	5.5 Case studies in Engineering	**T:24.1 - 24.4**	
6. Ordinary Differential Equations: Initial Value Problems	6.1 Euler's method and error analysis, improvements of Euler's method	**T:25.1 - 25.2**	To apply numerical techniques for solving first order ODEs To develop the code/algorithm using MATLAB
	6.2 Runge Kutta Methods	**T:25.3**	
	6.3 System of Equations	**T:25.4**	
	6.4 Adaptive Runge Kutta Methods	**T:25.5**	
	6.5 Computer Algorithm for solving ODEs using MATLAB	**T: 25**	
	6.6 Stiffness	**T: 26.1**	
7. Ordinary Differential Equations: Boundary Value Problems	7.1 Shooting Method	**T: 27.1.1**	To apply numerical techniques for solving 2^{nd} order ODEs To develop the code/algorithm using MATLAB
	7.2 Finite Difference Method	**T: 27.1.2**	
	7.3 Computer Algorithm for solving ODEs using MATLAB	**T: 27.3**	
	7.4 Case studies in Engineering	**T:28.1 - 28.4**	

8. Partial Differential Equations	8.1 PDE's and Engineering Practice, Elliptic PDE's: Laplace equation and solution	**T:29.1 - 29.2**	To apply numerical techniques for solving PDEs To develop the code/algorithm using MATLAB
	8.2 Boundary Conditions	**T:29.3**	
	8.3 Parabolic equation, Heat conduction equation, Explicit and Implicit methods	**T:30.1 - 30.3**	
	8.4 Crank Nicholsan Method, ADI Method	**T:30.4 - 30.5**	
	8.5 Computer Algorithm for solving PDEs using MATLAB	**T:31.4**	
	8.6 Case studies -1	**T:32.1 - 32.2**	
	8.7 Case Studies - 2	**T:32.3 - 32.4**	

6. Evaluation Scheme:

Component	**Duration**	**Weightage (%)**	**Date & Time**	**Nature of component (Close Book/ Open Book)**
Mid-Semester Test	90 Min.	30		Open book
Comprehensive Examination	3 h	40	1/05/2021 FN	Open Book
Tutorial Tests*	10-15 minutes	15	During tutorial class hour	Open Book
Surprise Quiz #	10-15 minutes	10	During tutorial or regular class hours	Open Book
Assignment (application based)	1 week	5	Would be announced on 10th April and to be submitted by 20th April	Take Home

* Best 5 tut marks out of total 6 will be considered.
# 3 surprise quizzes would be conducted. No best of option.

7. Chamber Consultation Hour: Monday: 5:00 to 6:00 pm. Please email for making prior appointment.

8. Notices: would be displayed on Nalanda/Chemical Engineering Notice board

9. Make-up Policy: Make-up is granted only for genuine cases with valid justification and prior permission of Instructor-in-charge. No make up for tutorial test or surprise quiz.

10. Note (if any):

Instructor-in-charge
Course No. CHE F 242