BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI – GOA CAMPUS
INSTRUCTION DIVISION
SECOND SEMESTER 2018 – 2019
Course Handout (Part II)

Date: 8/01/2019

In addition to part – I (General Handout for all courses appended to the timetable), this portion gives further specific details regarding the course.

Course No.	**:**	**CHE F242**
Course title	**:**	**Numerical Methods for Chemical Engineers**
Instructor-in-charge	**:**	**Sharad Sontakke**
Tutorial Instructor	**:**	**Sharad Sontakke**

1. Scope and Objectives of the Course:

- Equation based modeling are used to predict behavior in several Chemical Engineering systems (both operations and processes). Many a time, these equations are not amenable to analytical solutions. In such cases, use of numerical methods is necessary which then provide a way for the engineer to translate the language of mathematics and physics into information that may be used 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. 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.

2. Text Book

"Numerical Methods for Engineers", Steven Chapra and Raymond Kanale, McGraw Hill, Sixth Edition.

3. Reference Books

1. Numerical Methods for Engineers, Santosh K Gupta, New Academic Science (September 15, 2012), 3rd Edition
2. Stefan J. Chapman "MATLAB® Programming for Engineers", 3rd Ed. Thomson Learning

4. Course Plan:

Lec. No.	Learning Objectives	Topics to be covered	TB / RB
1	Introduction	Introduction to the course, Concept of simple mathematical model and conservation laws, Role of programming and softwares	TB Chap 1 (1.1 – 1.2) TB Chap 2
2-3	Error analysis	Significant digits, error definitions, Concept of iterative calculations, Round off errors, Computer representation of numbers, Arithmetic manipulations of computer numbers; Taylor series and its use in truncation error estimation, Propagation of errors and total numerical error, blunders, formulation errors and data uncertainty	TB Chap 3 (3.1 – 3.4) TB Chap 4 (4.1 – 4.4)
4 – 7	Roots of equations (Bracketing methods)	Roots of equations and Engineering practice, introduction to graphical method for finding root, Bisection method & False Position methods, Incremental searches and initial guess	TB Chap 5 (5.1 – 5.4)
8 –10	Roots of equations (Fixed point methods)	Single point Iteration, Newton Raphson method, Secant method, Multiple roots and system of non-linear equations	TB Chap 6 (6.1 – 6.6)
11 – 13	Roots of Polynomials	Polynomials in Engineering, Computing with polynomials, Muller and Bairstow's method, Case studies in Engineering	TB Chap 7 (7.1 – 7.7) TB Chap 8
14 – 15	Linear Algebraic equations	Linear algebraic equations and Engineering practice, Gauss Elimination, Naïve Gauss elimination, pitfalls, Techniques for improving solutions	TB Chap 9 (9.1 – 9.4)
16 – 17	Linear Algebraic equations	Gauss Jordan method, LU Decomposition and Matrix Inversion methods	TB Chap 9 (9.7) TB Chap 10 (10.1 – 10.3)
18 – 19	Linear Algebraic equations	Special Matrices, Gauss Seidel method, Case studies in Engineering	TB Chap 11 (11.1 – 11.3) TB Chap 12
20	Curve fitting (Least squares regression)	Curve fitting and Engineering Practice, Least square fit of straight line, Linearization of non-linear relationships	TB Chap 17 (17.1- 17.1.6)

21	Curve fitting (Least squares regression)	Polynomial regression, Multiple linear regression, Non-linear regression	TB Chap 17 (17.2, 17.3, 17.5)
22 – 23	Curve fitting (Interpolation)	Divided difference Interpolation formula, Lagrange's interpolation, Spline interpolation, Case studies	TB Chap 18 (18.1, 18.2, 18.6) Chap 20
24 – 25	Numerical Integration	Role in Engineering, Newton Cotes formula, Trapezoidal rule, Simpson's 1/3 and 3/8 rule, Unequal segment Integration, Multiple integrals	TB Chap 21 (21.1 – 21.5)
26 – 27	Numerical Differentiation	High accuracy differentiation formulas, Case studies in Engineering	TB Chap 23 (23.1) TB Chap 24
28 – 29	Ordinary Differential equations (ODE)	ODE's and Engineering Practice, Euler's method and error analysis, Runge Kutta methods (2^{nd} and Higher order), System of ODE's, Adaptive Runge Kutta method	TB Chap 25 (25.1 – 25.5)
30 – 31	Ordinary Differential equations (ODE)	Concept of stiffness, Multistep methods (Non-starting Heun's method)	TB Chap 26 (26.1 – 26.2.2)
32 – 34	Ordinary Differential equations (ODE)	Methods for Boundary value problems, Eigen value problems, Case studies in Engineering	TB Chap 27 (27.1 – 27.2.5)
35 – 36	Partial Differential equations (PDE)	PDE's and Engineering Practice, Elliptic PDE's, Laplace equation and solution technique, Introduction to control volume approach	TB Chap 29 (29.1 – 29.4)
37 – 38	Partial Differential equations (PDE)	Parabolic equation, Heat conduction equation, Explicit and Implicit methods	TB Chap 30 (30.1 – 30.4)
39 – 40	Partial Differential equations (PDE)	Introduction to finite element method (1 – D problem only), Case studies in Engineering	TB Chap 31 (31.1 – 31.2) TB Chap 32

5. Evaluation Scheme:

Component	Weightage (%)	Date
Attendance	10	Regular basis
Quizes/Assignments*	20	To be announced by IC
Mid-Sem Exam	30	As per the timetable
Comprehensive Exam	40	As per the timetable

(* : This will be strictly subject to your attendance in the class in which assignment/ class assignment/ quiz is announced/ conducted)

Note:

- Chamber consultation hours: Thursday 4 to 5 pm.
- Make-up will be granted for genuine cases only. Prior permission of IC is compulsory.

Instructor-Incharge
CHE F242