BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI – PILANI CAMPUS
INSTRUCTION DIVISION
SECOND SEMESTER 2015 – 2016
Course Handout (Part II)

Date: 07.01.2016

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	:	**ARVIND KUMAR SHARMA**
Instructor	:	**Ajay Kumar Pani & Tapas Kumar Patra**

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 Objectives

Equation based modeling is 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 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. Numerical methods for differentiation and integration and curve fitting techniques will also be covered. Strong emphasis will be placed on problem solving based on case studies in engineering. The role of computers and softwares along with identification, quantification and minimization of errors involved in numerical analysis will also be highlighted.

3. Text Book (TB)

Chapra, S. C. and R. P. Canale, *Numerical Methods for Engineers*, 6th Edition, McGraw Hill Education (India) Pvt. Ltd., New Delhi, 2010 [MHE (I) Ed. 2012, 3rd Reprint 2013] (or higher edition if available!).

4. Reference Book (RB)

1. Gupta, S. K., *Numerical Methods for Engineers*, 3rd Edition, New Age International (P) Ltd., New Delhi, 1995! (Computer-set ed. 2015 or higher edition if available!).
2. Chapra, S. C., *Applied Numerical Methods with* MATLAB^R *for Engineers and Scientists*, 3rd Edition, McGraw Hill Education (India) Pvt. Ltd., New Delhi, 2012 (4th Reprint 2013) [or higher edition if available!].

5. Course Plan

Lecture No.	Learning Objectives	Topics to be covered	TB / RB
1	Modeling and Computers	Introduction to the course, Concept of simple mathematical model and conservation laws, Role of programming and softwares (only an introduction)	TB Chap 1 (1.1 – 1.2) TB Chap 2
2 – 3	Error analysis	Significant digits, accuracy, precision, error definitions, Concept of iterative calculations, Round off errors, Computer representation of numbers, Arithmetic manipulations of computer numbers	TB Chap 3 (3.1 – 3.4)
4 – 5	Error analysis	Taylor series and its use in truncation error estimation, Propagation of errors and total numerical error, blunders, formulation errors and data uncertainty	TB Chap 4 (4.1 – 4.4)
6 – 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 – 9	Roots of equations (Fixed point methods)	Single point Iteration, Newton Raphson method, Secant method, Brent's method, Multiple roots and system of non-linear equations	TB Chap 6 (6.1 – 6.6)
10 – 13	Roots of Polynomials	Polynomials in Engineering, Computing with polynomials, Muller and Bairstow's methods, Using Excel to determine roots, 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, Using Excel to solve linear equations, Case studies in Engineering	TB Chap 11 (11.1 – 11.3) TB Chap 12
19 A !	Optimization	A brief, but judicious discussion of topics … !	TB Chaps 13-16
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) TB Chap 28
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

6. Evaluation Scheme*

Components		Duration	Weightage (%)	Marks	Date & Time	Nature **
1	Mid Sem. Test	1.5 hr.	30	90	16/3 9:00 - 10:30 AM	CB + OB
2#	Tutorial Tests / Surprise Quizzes / Assignments / Projects … *etc.*	-	30	90	-	CB/OB
3	Comprehensive Exam.	3 hr.	40	120	7/5 FN	CB + OB

* **If any change in this / rest of the handout : it will be communicated in Classes / Tutorials – pls follow them.**
** **CB** = Close Book **OB** = Open Book
# A judicious blend of these components will spread over class and tutorial hours. There will not be "best of option" in assignments and / or projects. In case of tutorial tests and/or surprise quizzes, all possible efforts will be made so that "best of option" may be exercised.

- **Chamber consultation hour** will be announced in the class.
- The **notices,** if any**,** concerning the course, will be displayed on the notice board of the Department of Chemical Engineering **only**.
- **Make-up** will be granted for **genuine cases only**. Certificate from authenticated doctor, say from the Medical Center, must accompany make-up application (*only prescription or vouchers for medicines will not be sufficient*). Prior permission of IC is compulsory.

Instructor-in-charge | CHE F242