BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI, PILANI CAMPUS INSTRUCTION DIVISION

First Semester 2016-2017 Course Handout (Part-II)

Date: 02/08/2016

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 G523

Course Title : Mathematical Methods in Chemical Engineering

Instructor-in-Charge : PRATIK N SHETH

1. Course Description:

An introduction to mathematical modeling and simulation, Fundamentals of functional analysis, Linear algebraic equations and related numerical schemes, ODE's IVP and related numerical schemes, Partial differential equations and related numerical schemes, Optimization and related numerical schemes, Application of the above principles to solving problems in Chemical Engineering, Role of computer programming and packages in problem solving

2. Scope & Objective:

Mathematical methods play a key role in understanding the concepts and analyze the chemical processes. The detailed understanding on how to apply different kinds of mathematical methods for various theories related to transport phenomena, reaction engineering and process control is essential. Analytical and Numerical, both approaches are required to be understood to solve any set of equations which may represent any process model of chemical engineering. The present course aims to help the student to learn, different mathematical technique to solve and analyze different classes of problems.

2.Text Books:

- 1. S. Pushpavanam, "Mathematical Methods in Chemical Engineering," Prentice-Hall-India, New Delhi, 1998.
- 2. Santosh K Gupta, Numerical Methods for Engineers, 2nd Edition, New Age International Publishers, New Delhi, 2010

3. Reference Books:

- 1. P S Ghoshdastidar, "Computer Simulation of Flow and Heat Transfer", Tata McGraw-Hill Publishing Company Limited, New Delhi, 1998.
- 2. Curtis F Gerald and Patrick O Wheatley, "Applied Numerical Analysis", Pearson Education, Inc., Delhi., 2004

4. Course Plan:

| Lecture No. | Learning Objectives | Topics to be covered | Reference Chap./ Sec. (Book) |
|----------------|--------------------------|--|---------------------------------|
| 1 | Models in Chemical Engg. | Modeling, Simulation, Types of Equation | Ch. 1 (T1) |
| 2-7 | Vector & Vector Spaces | Vectors, Metrics, Norms, Inner Products, Normed linear space. Dimension of Vector spaces, Applications, Gram-Schmidt Ortho- normalisation. | Ch. 2 (T1) |

| 8-10 | Matrices, Operators & Transformations | Matrices, Eigenvalues, Eigen vectors, Rayleigh's Quotient | Ch. 3 (T1) |
|-------|--|---|---|
| 11-15 | Application of Mathematics to Chemical Engg. System | Linear Algebric Eq. ODE, IVP, Non Self adjoint systems. | Ch. 4 (T1) |
| 16-19 | Numerical solutions of ODE'S (BVPS) | Finite difference technique. Orthogonal collocation technique. | Ch. 6: 6.1 – 6.4 (T2) |
| 20-22 | Applications of Numerical Solution for ODE (BVP) | One dimensional Steady State Heat Conduction | Ch. 4: 4.1 -4.7 (R1) Or Ch. 6: 6.7 (R2) |
| 23-24 | Partial Differential Equation | Classification of PDE, boundary conditions, Developing PDE in Chemical Engg. Systems. | Ch. 5 (T1) |
| 25-27 | Numerical solutions of PDE'S | Classification of PDEs. Initial and Boundary conditions. Finite difference technique orthogonal collocation technique. | Ch. 7:7.1-7.4 (T2) |
| 28-31 | Application of Numerical solutions of Elliptic Equation | Two Dimensional Steady State Heat Conduction | Ch. 4: 4.8 (R1) Or Ch.8: 8.1 (R2) |
| 32-35 | Application of Numerical solutions of Parabolic Equations | Transient One/Two/Three dimensional Heat Transfer Conduction | Ch. 4: 4.9-4.28 (R1) Or Ch.8: 8.2 (R2) |
| 34-36 | Application of Numerical solutions of Hyperbolic Equations | Solution of Vibrating String Problem: Wave Equation | Ch.8: 8.3 (R2) |
| 37-38 | Introduction to Finite Element Analysis | Introduction to Finite Element Methods | Ch. 9:9.1(R2) |
| 39-40 | Finite Elements for ODE | Application of FEA to ODEs | Ch. 9:9.2(R2) |
| 41-42 | Finite Elements of PDE | Application of FEA to PDEs | Ch. 9:9.3(R2) |

5. Evaluation Scheme:

| Component | Duration | Weightage | Date & Time | Remarks |
|------------------|----------|-----------|--------------------|----------------------------|
| Mid Semester | 90 min | 25 | | СВ |
| Test | | | <test_1></test_1> | |
| Assignments | | 20 | To be announced in | Take home type or |
| (4 No.) | | | the class | During regular class hours |
| | | | | (Open book) |
| Projects (2 No.) | | 20 | | Based on C/MATLAB |
| | | (8+12) | | programming |
| Comprehensive | 3 hours | 35 | <test c=""></test> | CB+OB |
| Exam. | | | TEST_C> | |

- **6. Chamber Consultation Hour:** To be announced in the class.
- **7. Notices:** All notices concerning this course will be displayed on the Chemical Engineering Notice Boards
- **8. Make-up Policy:** Make-up is granted only for genuine cases with valid justification and prior permission of Instructor-in-charge.