Birla Institute of Technology & Science, Pilani
Hyderabad Campus

Second Semester 2019-2020

Course Handout (Part-II)

Date: 06//01/2020

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 F 242**
Course Title: **Numerical Methods for Chemical Engineers**
Instructor-in-Charge: **Dr. Vikranth Kumar Surasani**
Instructors: **Dr. Vikranth Kumar Surasani**

Scope &Objective:

With the increase in the computational power and the wide spread availability of computers (esp. PCs), Numerical methods evolved as a tool to address many complex physic-chemical phenomena. Today, numerical methods are powerful tools to solve complex problems of engineering and environmental systems etc. The techniques of Numerical Methods must be complemented with any computer programming that converts the system of equations into simple arithmetic operations. Many commercial tools Ansys Fluent, Aspen, MatLab and etc are based on these numerical techniques written in the form of algorithms and functions. In this course you will be learning about the mathematical background behind the Numerical Methods, the detailed knowledge of numerical techniques and programming the numerical methods with Matlab.

Course Outcomes:

CO1. You should embark on the study of Numerical methods such as Solution to Linear System, ODEs and PDEs
CO2. The role of computers & Programming in implementing numerical methods for solving Engineering problems and Design of new methods. You be dealing with Matlab as a part of this course for programming numerical methods and for the data visualization.
CO3. You will be able to generate to solving any physio-chemical processes which is a part of the system or a system as whole.
CO4. You will be learning the basics behind the most of the commercial tools using for numerical simulation

Generic Program Outcomes: Program Outcomes(POs) 3(a) through 3(k) plus any additional outcomes that may be articulated during the course.

PO1. 3(a) an ability to apply knowledge of science and engineering.
PO2. 3(b) an ability to design and conduct safety demonstration experiments, as well as to analyze and interpret results.
PO3. 3(c) an ability to design a safety based component, or process to meet desired needs within realistic constraints such as economic, environmental, social, ethical, health and sustainability.
PO4. 3(d) an ability to function on teams.
PO5. 3(e) an ability to identify, formulate, and solve engineering problems.
PO6. 3(f) an understanding of professional and ethical responsibility.
PO7. 3(g) an ability to communicate effectively.
PO8. 3(h) the broad education necessary to understand the impact of engineering solutions in a global, economic, environmental, and societal context
PO9. 3(i) a recognition of the need for, and an ability to engage in life-long learning
PO10. 3(j) a knowledge of contemporary issues
PO11. 3(k) an ability to use the techniques, skills, and modern engineering tools necessary for engineering practice.

Text Books:

TB1 Steven C Chapra, Raymond P Canale, “Numerical Methods for Engineers”, Tata McGraw-Hill Special Indian 5th Edition 2007.

Reference Books:

RB1 Stefan J. Capmann "Matlab Programming for Engineers", 4th Ed. Cengage Learning. (Available from Books 24x7)

Numerical Tools: NT1 Matlab NT2 Excel

Course Plan:

Lec. No.	Learning Objectives	Topics to be covered	Chapter in the Text Book
1	Modeling and Computers	Introduction to the course; Concept of simple mathematical model and conservation laws; Role of programming and software.	TB Chap 1 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; Taylor series; Truncation error estimation, Propagation of errors and total numerical error, blunders, formulation errors and data uncertainty;	TB Chap 3 Chap 4
4-6	Linear Algebraic equations	Linear algebraic equations and Engineering practice; Gauss Elimination; Naïve Gauss elimination; pitfalls, Techniques for improving solutions.	TB Chap 9
7-9	Linear Algebraic equations	Gauss Jordan method; LU Decomposition and Matrix Inversion methods; Special Matrices, Gauss Seidel method; Case studies in Engineering	TB Chap 9,10,11,12
10-13	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
14	Ordinary Differential equations (ODE)	Concept of stiffness, Multistep methods (Non-starting Heun's method)	TB Chap 26
15-16	Ordinary Differential equations (ODE)	Methods for Boundary value problems, Eigen value problems, Case studies in Engineering	TB Chap 27
17	Roots of equations (Bracketing methods)	Engineering practice; Introduction to graphical method; Bisection method; False Position methods; Incremental searches and initial guess.	TB Chap 5
18-19	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
20-22	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
23 – 25	Numerical Differentiation	High accuracy differentiation formulas, Case studies in Engineering	TB Chap 23,24
26 – 27	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
28– 30	Partial Differential equations (PDE)	Parabolic equation, Heat conduction equation, Explicit and Implicit methods; Case studies in Engineering	TB Chap 30
31-32	Curve fitting (regression)	Curve fitting and Engineering Practice, Least square fit of straight line, Linearization of non-linear relationships	TB Chap 17
33-34 35–36	Curve fitting (regression)	Polynomial regression, Multiple linear regression, Non-linear regression	TB Chap 17
	Curve fitting (Interpolation)	Divided difference Interpolation formula, Lagrange's interpolation, Spline interpolation, Case studies	TB Chap 18,20
37 - 40	Case Studies	Some examples of Optimization and Complex Chemical Engineering problem solutions.	

***Tutorial & Class Tests/Submissions:**

S. No.	Learning Objective	Topic
1-2	Introduction to MatLab	Graphical Interface; Variables Types; Vectors & Matrices Writing Script file; Plot tools;
2	Vector operations using Matlab	Linear Regression Example
3	Matrices and operations	Built in functions; Writing functions; Control structures; Managing variables;
4	Sol. to Linear System Solution	Direct and Iterative methods
5	Sol. to Non-Linear System Solution	Jacobi-Method
6	Ordinary Differential Eqs.-11	Eulers Approximations
7	Ordinary Differential Eqs-2	Higher Order Methods & R-K Methods
8	Partial Differential Equations-1	Eliptical Problems
9	Partial Differential Equations-2	Parabolic Problems
10	Partial Differential Equations-2	Plug flow, tracer Test & Break through curves

*Topics may not be limited as the mentioned in table

Evaluation Scheme:

EC No.	Evaluation Component	Duration	Weightage (%)	Date& Time	Nature of Component
1.	Midterm	90min	30	4/3 1.30 -3.00 PM	CB(10%)+OB(15%) (MATLAB Required)
3.	Comprehensive	3 hrs.	40		CB(10%)+OB(30%) (MATLAB Required)
4.	Quizzes/Surprise tests	--	10		CB (MATLAB Required)
5.	Tutorial+ Assignments*	--	20	08/05 FN	OB (MATLAB Required)

*All Open book assignments are based on Matlab programming. You should utilize CAD Lab hrs to complete assignments.

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

CAD Lab Practice Hours: 5-8 pm (All days)

Chamber Consultation Hour: 5-5:30 pm (Mon, Wed, Friday)

Notices: All notices concerning this course will be displayed on the Chemical Engineering Notice Board and Course Management System(CMS)portal.

Make-up Policy: Make-up is granted only for genuine cases having 75 % attendance with valid justification. A prior permission from the Instructor-in-charge is required.

Instructor-in-charge
(Dr. Vikranth Kumar Surasani)
CHE F242