

**Second Semester 2022-2023**

Course Handout (Part-II)

##### Date: 16//01/2023

**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: Prof. Vikranth Kumar Surasani**

**Instructors: Prof. 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:**

1. You should embark on the study of Numerical methods such as Solution to Linear System, ODEs and PDEs
2. 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.
3. You will be able to generate to solving any physio-chemical processes which is a part of the system or a system as whole.
4. You will be learning the basics behind the most of the commercial tools using for numerical simulation

**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** | **TB /NT** |
| 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; Naive 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 (2nd 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 | 14/03 9.30 - 11.00AM | CB(10%)+OB(20%)  (MATLAB Required) |
| 3. | Comprehensive | 3 hrs. | 45 | 10/05 FN | CB(10%)+OB(35%)  (MATLAB Required) |
| 4. | Quizzes/Surprise tests | -- | 10 |  | CB  (MATLAB Required) |
| 5. | Tutorial+ Assignments\* | -- | 15 |  | OB  (MATLAB Required) |

\*All Open book assignments are based on Matlab programming. You should utilize CC 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.

**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.

###### Instructor-in-charge

###### (Prof. Vikranth Kumar Surasani)

###### CHE F242