NUMERICAL METHODS AND APPLICATIONS IN CHEMICAL ENGINEERING

Course Code: 22CH1107

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Course Outcomes: At the end of the course the student shall be able to

CO1: Solve a system of linear algebraic equations using Gauss elimination, Gauss-Siedel and LUdecomposition methods. (L3)

CO2: **S**olve linear/nonlinear algebraic and transcendental equations using numerical methods (L3)

CO3: **A**pply curve fitting techniques to approximate a function in interpolating and extrapolating a givendata. (L2)

CO4: **S**olve ordinary differential equations by Euler's method and Runge Kutta method. (L3)

CO5: **A**pply numerical methods to boundary value problems and partial differential equations. (L3)

UNIT-I **10 Lectures**

Matrix Operations

Elementary row transformations - Rank, Eigen Values, Solution of system of linear equations by Gauss elimination, Gauss-Seidel and LU decomposition methods.

Learning outcomes: After the completion of the Unit I, the student will be able to

1. Determine the rank of a matrix using row transformations.(L3)
2. determine eigenvalues for a given matrix.(L3)
3. solve the system of linear algebraic equations using Gauss elimination, Gauss Siedel and LU decomposition methods (L3)

UNIT-II **10 Lectures**

Root Finding

Solution of Nonlinear Algebraic Equations: Introduction, Solving one variable and two variable nonlinear problems using Newton-Raphson. Chemical engineering problems involving solution of linear and Non-linear algebraic equations like calculation of friction factor in turbulent flows, calculating optimum insulation thickness, chemical reaction equilibria calculations for two equilibrium reactions.

Learning outcomes: After the completion of the Unit II, the student will be able to

1. determine the Newton-Raphson formula for one and two variable cases. (L3)
2. solve one variable and two variable nonlinear problems(L3)
3. apply Newton-Raphson method to chemical engineering problems. (L3)

UNIT-III **10 Lectures**

Regression Analysis. Model Building through Interpolation and Extrapolation

Regression Analysis: Introduction, least squares curve-fitting methods, Lagrangian Interpolation (Unequal Intervals)

Numerical Differentiation and Integration

Numerical differentiation: Three point Lagrangian formulae.

Numerical Integration: Trapezoidal rule, Simpson’s 1/3 rule, Chemical engineering problems involving numerical differentiation and integration.

Learning outcomes: After the completion of the Unit III, the student will be able to
1. modal the curve fitting (Straight line, second degree curve, exponential curve and power curve) using the method of least squares. (L3)
2. perform interpolation using Lagrange's formulae. (L3)
3. evaluate numerical derivative using three point formulae. (L5)
4. perform numerical integration using Trapezoidal rule, Simpson's 1/3 rule. (L3)

UNIT-IV **10 Lectures**

Numerical Solution of Ordinary differential equations (Initial Value problems)

Solution of ordinary Differential Equations- Introduction to Ordinary Differential Equations, Initial and boundary value problems, Implicit and Explicit Euler method, Runge-Kutta 4^{th} order method, Chemical engineering problems involving single, and a system of ODEs.

Learning outcomes: After the completion of the Unit IV, the student will be able to
1. solve initial value ordinary differential equations by Euler's method, and Runge Kutta methods.(L3)
2. differentiate Implicit and Explicit Euler methods. (L4)
3. explain the advantages of Runge Kutta method over Euler method. (L2)
4. apply Euler's method, and Runge Kutta methods to chemical engineering problems. (L3)

UNIT-V **10 Lectures**

Numerical Solution of Boundary Value problems and Partial differential equations

Introduction to finite difference methods (FDM). Methods of handling Dirichlet, Neumann and Robin boundary conditions, handling flux boundary conditions on the right and left boundaries.

Formulating chemical engineering problems like steady state heat transfer in a slab with Dirichlet, Neumann and Robin boundary conditions.

Introduction to partial differential equations: elliptic, parabolic & hyperbolic equations and their applications in chemical engineering. Classification of chemical engineering problems into elliptic, parabolic & hyperbolic equations.

Formulating an unsteady state heat transfer problem in a slab using FDM in space and integrating along time using Runge Kutta 4^{th} order method.

Learning outcomes: After the completion of the Unit V, the student will be able to
1. solve boundary value problems using finite difference methods.(L3)
2. classify partial differential equations. (L4)
3. solve partial differential equations using finite difference methods. (L3)

Text Books:

1. S.K. Gupta, *Numerical methods for Engineers*, New Age International (P) Limited, Publishers, 1998
2. S.S. Sastry, *Introductory Methods of Numerical Analysis*, 5^{th} Edition, PHI publisher, 2012.

References:

1. Ajay K. Roy, *Mathematical methods in Chemical and Environmental Engineering*, Thomson Learning, 2000
2. Erwin Kreyszig, *Advanced Engineering Mathematics*, Wiley India, 10^{th} edition, 2011.