NUMERICAL METHODS IN CHEMICAL ENGINEERING

COURSE CODE:15CH1118

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COURSE OUTCOMES:

At the end of the course the student shall be able to

CO 1 Recognize the importance of numerical methods in engineering and be able to solve the roots of non linear algebraic equations

CO 2 Apply Gauss elimination, LU decomposition and Gauss-Jordan methods to solve simultaneous linear equations.

CO 3 Calculate the least squares method and do linear and non linear regression.

CO 4 Apply finite difference techniques to handle boundary value problems.

CO 5 Classify partial differential equations and apply finite difference techniques to solve them.

UNIT-I (13 LECTURES)

Introduction and Importance of Numerical methods, Taylor series expansion of functions of single and two variables.

Finding the roots of a single variable functions by bisection, interval halving and Newton - Raphson methods.

Finding the optimum insulation thickness. Calculating volumes using cubic Equation of State, Flash calculations.

Finding the roots of a two variable function by Newton - Raphson method.

Solution of calculating pressure drop and friction factor in turbulent flows.

Calculating the extent of reactions for two equilibrium reactions. Numerically calculating derivatives.

UNIT-II (7 LECTURES)

Solution of Linear simultaneous equations by Gauss Elimination and LU decomposition, Gauss Jordan elimination.

Solution of a Heat transfer composite slab.

UNIT-III (8 LECTURES)

Linear Least squares method. Non Linear regression.

Function fitting using Lagrange Interpolation, Pade approximation.

Example of fitting specific heat capacity and thermal conductivity with temperature. Fitting Activity coefficients for non-ideal solutions and develop equation for excess Gibbs free energy.

UNIT-IV (14 LECTURES)

FINITE DIFFERENCING SCHEME:

Backward, Central and Forward Schemes. One sided and image schemes to handle boundary conditions.

ORDINARY DIFFERENTIAL EQUATIONS:

Initial Value problems, Implicit and Explicit Euler methods, Fourth order Runge-Kutta method.

Solution of unsteady Heat transfer problem treated as lumped system.

Time need to heat a mass of liquid from an initial temperature to final temperature.

BOUNDARY VALUE PROBLEMS:

Introduction to shooting method to convert a BVP to IVP.

Solution of a BVP using central differencing method: 1 D steady state heat conduction in slab.

UNIT-V (8 LECTURES)

Partial differential equation (PDE):

Classification of PDE’s and boundary conditions. Illustration of finite difference schemes to solve the two dimensional Heat conduction problem. One dimensional unsteady state heat conduction problem:

Finite differencing in space and using Runge Kutta for integrating in time.

TEXT BOOKS:

1. Gupta, S.K. "Numerical Methods for Engineers", Tata McGraw Hill, 2010.

REFERENCES:

1. Mark.E.Davis, "Numerical Methods and Modeling for Chemical Engineers", 1st Edition, willey, 1984.