

UG

Course Code: CH211

Credit: 2

Version: 1

Prerequisite Course: Nil

Department: **Chemical Engineering**

Course Name: **Numerical Methods in Chemical Engineering**

L-T-P: **2-0-0**

Approved on:

Linear Algebraic Equations: Introduction, Gauss-Elimination, Gauss-Siedel and LU Decomposition methods, Thomas' algorithm.

Eigen Values and Eigen Vectors of Matrices: Introduction, Fadeev-Leverrier's method, Power method, Householder's and Givens' method.

Nonlinear Algebraic Equations: Single variable and multivariable successive substitution method, single variable and multivariable Newton-Raphson technique, Polynomial root finding methods.

Function Approximation: Least squares curve fit, Newton's interpolation formulae, Lagrangian interpolation, Pade approximation, Cubic spline approximation. Integration formulae: Trapezoidal rule, Simpson's rule.

Ordinary Differential Equations - Initial Value Problems: Explicit Adams-Bashforth technique, Implicit Adams-Moulton technique, Predictor-corrector technique, Runge-Kutta methods, Stability of algorithms.

Ordinary Differential Equations - Boundary Value Problems: Finite difference technique, Orthogonal Collocation (OC), Shooting Techniques.

Partial Differential Equations: Partial Differential Equations (PDE) - Classification of PDE, Finite difference technique (Method of lines), Orthogonal collocation. Case Studies. Use of spreadsheets and MATLAB in Chemical Engineering.

Books

1. Gupta, S. K., "Numerical Methods for Engineers," New Age International Ltd., New Delhi, 1995.
2. Constantinides, A., and Mostoufi, N., "Numerical Methods for Chemical Engineers with MATLAB Applications," Prentice Hall, 1999.
3. Hanna, O.T. and Sandall, O.C., "Computational Methods in Chemical Engineering," Prentice-Hall, 1995.
4. Davis, M.E., "Numerical Methods & Modeling for Chemical Engineers," John Wiley, 1984.
5. Press, W. H., Teukolsky, S. A., Vetterling, W. T., Flannery, B. P., "Numerical Recipes in C," 2nd ed., Cambridge University Press, New Delhi, 1992.