7th Semester	RCH7D002	Computer Application in Chemical Engineering	L-T-P 3-0-0	3Credits

Module-I   8 hrs

Review of solution methods of nonlinear single variableequations, polynomials (determination of quadratic factors),linear set of simultaneous equations, ill conditioned matrix, andset of nonlinear equations using Newton's and globallyconvergent methods, Solution of homogeneous set of linear equations using eigenvalues and eigen vectors with application to chemicalengineering problems.

Module-II   4 hrs

Review of numerical differentiation and numerical integrationmethods, quadratures and their applications to numericalintegration.

Module-III   8 hrs

Review of single step and multiple step methods to solve initialvalue ordinary differential equations problems, estimation oferror and its propagation in single step and multiple stepmethods, step size selection and adaptable step size Runga-Kuttamethods, stiff ODE's and Gear's class of methods.

Module-IV   7 hrs

Boundary value problems (BVP) - shooting methods for linearsystem, finite difference methods, regular perturbation method,method of weighted residuals and orthogonal collection methodsto solve first and higher order BVP in ODE's application tochemical engineering systems, concept of finite element.

Module-V   9 hrs

Review of finite difference techniques to solve partial differenceequations (PDE's), similarity transformation, method ofweighted residuals, orthogonal collocation to solve PDEs withtheir application to chemical engineering systems.

Books:

1. Finlayson B. A., "Introduction to Chemical EngineeringComputing", 7thEd.., Wiley Interscience publication.

2. Gerald C. F. and Wheatly P. O.; "Applied Numerical Analysis",7thEd., Addison Wesley.

3. Rice R.G. and Do D. D., "Applied Mathematics for ChemicalEngineers", Wiley.

4. Beers K. J., "Numerical Methods for Chemical Engineering:Applications in Matlab", Cambridge University Press.

5. Constantinides A. and Mostoufi N., "Numerical Methods forChemical Engineers with MATLAB Applications", Prentice Hall.

6. Cutlip M. B. and Shacham M.., "Problem Solving in Chemical andBiochemical Engineering with POLYMATH, EXCELL andMATLAB", 2ndEd., Prentice Hall.