INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR

1. **Name of the Academic Unit: Chemical Engineering**

2. **Subject Name: Computer Aided Process Engineering**
   L-T-P: 3-1-0 Credits: 4

3. **Pre-requisites: None**

4. **Syllabus and reference books:**

Syllabus

Analytical and numerical (direct and indirect) methods for linear algebraic equation systems; Iterative convergence methods and their applications in process engineering; Numerical methods for ODE-IVP and ODE-BVP systems with chemical process examples; Numerical methods for processes with PDEs; Convergence and stability analysis of chemical processes; Numerical simulation of multivariable and differential algebraic equation (DAE) systems; Method of least-squares; Polynomial interpolation; Numerical integration; Process optimization; Flowsheet simulator like ASPEN; Application of AI in process engineering.

Reference Books

1. Ramirez, W.F. (1997). *Computational methods for process simulation*, 2nd ed., Reed Educational and Professional Publishing Ltd., Oxford.
2. Bequette, B.W. (1998). *Process dynamics, modeling, analysis, and simulation*, 1st ed., Prentice-Hall, Upper Saddle River, New Jersey.
3. Gupta, S.K. (2003). *Numerical methods for engineers*, 1st ed. (reprinted version), New Age International (P) Ltd., New Delhi.
4. Luyben, W.L. (1990). *Process modeling, simulation, and control for chemical engineers,* 2nd ed., McGraw-Hill Book Company, Singapore.

5. **Lecture-wise break-up:**

Sl. No.	Topic	No. of lectures
1.	**Introduction to computer aided process engineering** Analytical vs. numerical methods, process modeling and simulation, definition of error and its various forms, examples	1
2.	**System of linear algebraic equation** Method: Analytical and numerical (direct and indirect) method Process example: steady state reactor and separator	3

3.	**System of nonlinear algebraic equation** Method: Iterative convergence methods (bisection, secant, false position, Newton, Muller, Chebyshev) and convergence analysis Process example: heat exchanger, flash drum	7
4.	**System of ODE: initial value problem (ODE-IVP)** Method: Euler, Heun, RK family, Adams-Bashforth-Moulton methods, and Convergence and stability analysis Other system: Stiff systems, Multivariable and differential algebraic equation systems Process example: batch reactor, CSTR, fed-batch bioreactor, adsorption, liquid-liquid extraction and distillation column	7
5.	**System of ODE: boundary value problem (ODE-BVP)** Method: Finite difference and initial value (Shooting) methods Other system: Nonlinear and coupled BVPs Process example: steady state cooling fin, heat conduction in a slab, reaction-diffusion system	6
6.	**System of PDE** Method: Finite difference methods (e.g., method of lines, Dufort-Frankel, Crank-Nicholson) and stability analysis Other system: Coupled PDEs Process example: Nonlinear reaction-diffusion system, Nonisothermal PFR, double pipe heat exchanger	6
7.	**Method of least-squares** Method: Linear least-squares, least-squares for nonlinear and polynomial functions, nonlinear least-squares Process example: Data fitting for various processes	3
8.	**Polynomial interpolation** Method: Newton, Lagrange, Piecewise polynomial interpolation Process example: Data fitting to various processes	5
9.	**Numerical integration** Method: Newton-Cotes, Romberg integration, Gauss-Legendre quadrature Process example: batch reactor, isothermal CSTR	4
10	**Flowsheet simulation, process optimization and AI**	6 (= 2+2+2)
Total number of hours		48