GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL (COMPUTER AIDED PROCESS DESIGN) (16)

Numerical Methods in Chemical Engineering

SUBJECT CODE: 3713007

SEMESTER: I

Type of course: Core - I

Prerequisite:

Rationale:

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks				Total Marks
L	T	P	C	Theory Marks		Practical Marks		
				ESE(E)	PA (M)	PA (V)	PA (I)	
3	0	2	4	70	30	30	20	150

Content

Sl. No.	**Topic**	**Teaching Hours**	**Module Weightage (%)**
1.	**Unit-1: Equation Forms in Process Modelling:** Introduction and motivation, linear and nonlinear algebraic equation, optimization based formulations, Ordinary Differential Equations (ODE) - Initial Value Problems (IVPs) and Differential Algebraic Equations (DAEs), ODE - Initial Value Problems (IVPs) and Partial Differential Equations (PDEs), abstract model forms, fundamentals of vector spaces, generalized concepts of vector space, sub-space, linear dependence, concept of basis, dimension, norms defined on general vector spaces, norms defined on different vector spaces, Cauchy sequence and convergence, Cauchy-Schwartz inequality and orthogonal sets, Gram-Schmidt process and generation of orthogonal basis, orthogonal basis matrix norms, classification of problems in numerical analysis, polynomial approximations, Taylor series approximation, Necessary and sufficient conditions for unconstrained multivariate optimization, transformations and unified view of problems through the concept of transformations		
2.	**Unit-2: Interpolation & Curve Fitting**: Least square approximations, Formulation and derivation of weighted linear least square estimation, Geormtraic interpretation of least squares Projections and least square solution, Function approximations and normal equation in any inner product space, Model Parameter Estimation using linear least squares method, Generic equation forms in transformed problems. Linear and Polynomial Regression, Introduction to polynomial		

	interpolation, Polynomial and function interpolations, Lagrange Interpolating Polynomials, Spline Interpolation, Cubic Spline		
3.	**Unit-3:** Linear Algebraic Equations : System of linear algebraic equations, conditions for existence of solution - geometric interpretations (row picture and column picture), review of concepts of rank and fundamental theorem of linear algebra, Classification of solution approaches as direct and iterative, review of Gaussian elimination, Introduction to methods for solving sparse linear systems: Thomas algorithm for tridiagonal and block tridiagonal matrices, Block-diagonal, triangular and block-triangular systems, solution by matrix decomposition, Iterative methods: Derivation of Jacobi, Gauss-Siedel and successive over-relaxation methods, Convergence of iterative solution schemes: analysis of asymptotic behavior of linear difference equations using Eigen values, convergence of iterative solution schemes, Optimization based solution of linear algebraic equations, matrix conditioning, examples of well conditioned and ill-conditioned linear systems.		
4.	**Unit-4**: Nonlinear Algebraic Equations: Method of successive substitutions, derivative free iterative solution approaches, Secant method, Regulafalsi method and Wegsteine iterations, Modified Newton's method and Qausi-Newton method with Broyden's update, Optimization based formulations and Leverberg-Marquardt method, contraction mapping principle and introduction to convergence analysis.		
5.	**Unit-5:** Ordinary Differential Equations - Initial Value Problems (ODE-IVPs) :Introduction, Analytical Solutions of Linear ODE-IVPs, basic concepts in Numerical solutions of ODE-IVP: step size and marching, concept of implicit and explicit methods, Taylor series based and Runge-Kutta methods, Multi-step (predictor-corrector) approaches, Stability of ODE-IVP solvers, choice of step size and stability envelopes, stiffness and variable step size implementation, Introduction to solution methods for differential algebraic equations (DAEs),		
6	**Unit-6:** Ordinary Differential Equations – Boundary Value Problems (ODE-BVPs) : Method of least squares for solving ODE-BVP, Gelarkin's method and generic equation forms arising in problem discretization, Errors in Discretization, Discretization using approximation theory, finite difference method for solving ODE-BVPs with examples, finite difference method for solving PDEs with examples, , Orthogonal Collocations method for solving ODE-BVPs with examples, Orthogonal Collocations method for solving PDEs with examples, Single shooting method for solving ODE-BVPs		

References books:

- Gilbert Strang, Linear Algebra and Its Applications (4th Ed.), Wellesley Cambridge Press (2009).
- Philips, G. M.,Taylor, P. J. ; Theory and Applications of Numerical Analysis (2nd Ed.), Academic Press, 1996.

- Gourdin, A. and M Boumhrat; Applied Numerical Methods. Prentice Hall India, New Delhi, (2000).
- Gupta, S. K.; Numerical Methods for Engineers. Wiley Eastern, New Delhi, 1995.
- Linz, P.; Theoretical Numerical Analysis, Dover, New York, (1979).
- Gilbert Strang , Introduction to Applied Mathematics, Wellesley Cambridge Press (2009)

Course Outcome:

At the end of the course, the student will be able to:

1. Students should be able to solve system of linear algebraic equations.
2. Students should be able to do numerical integrations of functions.
3. Students should be able to fit relationship between two data sets using linear, non-linear regression.
4. Students should be able to calculate maxima/minima and functions.
5. Student should be able to design, simulate and optimise chemical engineering operations and processes.

List of Laboratory Experiments

1. Introduction to computation platform to be used for laboratory (C/C++/ MATLAB /SCILAB)
2. Applications of data Analysis tools and Plotting
3. Fitting experimental data to model
4. Solution of Linear Algebraic Equations using inbuilt solvers.
5. Implementation of algorithm for solution of Linear Algebraic Equations
6. Solution of non-Linear Algebraic Equations using inbuilt solvers.
7. Implementation of algorithm for solution of non-Linear Algebraic Equations
8. Application to solution of multi-component distillation.
9. Solution of ODE-IVP with inbuilt solvers for chemical engineering application.
10. Solution of ODE-BVP with inbuilt solvers for chemical engineering application.
11. Solution of PDE with inbuilt solvers for chemical engineering application.
12. Individual Coues project by each student implementing numerical solution of any chemical engineering process.