



GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: M.E. in Chemical Engineering

Level: Post Graduate Degree

Branch: Chemical Engineering

Course / Subject Code: ME01030011

Course / Subject Name: Mathematical and Statistical
Methods in Chemical Engineering

w. e. f. Academic Year:	2024-25
Semester:	1 st Semester
Category of the Course:	PCC

Prerequisite:	Engineering Mathematics
Rationale:	The increasing importance of numerical methods in various branches of science and engineering have led to enhanced demand for courses dealing with the techniques of numerical analysis as numerical methods give the solution of applied problems when ordinary analytical methods fail. It is therefore clear training in engineering would be incomplete without an adequate understanding of numerical methods. Statistics deals with the collection, presentation, analysis and use of data to make decisions, solve problems and design products and processes.

Course Outcome:

After Completion of the Course, Student will able to:

No	Course Outcomes
01	Solve system of linear algebraic equations
02	Fit relationship between two data sets using linear, non-linear regression.
03	Calculate maxima/minima and functions
04	Design, simulate and optimise chemical engineering operations and processes.

Teaching and Examination Scheme:

Teaching Scheme (in Hours)			Total Credits L+T+ (PR/2)	Assessment Pattern and Marks				Total Marks
L	T	PR	C	Theory		Tutorial / Practical		
				ESE (E)	PA / CA (M)	PA/CA (I)	ESE (V)	
3	0	2	4	70	30	20	30	150

Course Content:

Unit No.	Content	No. of Hours	% of Weightage
1.	Equation Forms in Process Modeling: Introduction and motivation, linear and nonlinear algebraic equation, optimization based formulations, Ordinary Differential Equations	5	12



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	(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.	Interpolation & Curve Fitting: Least square approximations, Formulation and derivation of weighted linear least square estimation, Geometric 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	7	12
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 tri-diagonal and block tri-diagonal 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.	8	13
4.	Nonlinear Algebraic Equations:	5	12



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	Method of successive substitutions, derivative free iterative solution approaches, Secant method, Regula-falsi method and Wegstein 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.	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 ODEIVP solvers, choice of step size and stability envelopes, stiffness and variable step size implementation, Introduction to solution methods for differential algebraic equations (DAEs)	10	15
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	10	12
Total		45	100

Suggested Specification Table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
7	12	35	10	6	0

Where R: Remember; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create (as per Revised Bloom's Taxonomy)

References/Suggested Learning Resources:



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(a) Books:

1. S C Chapra and R P Canale, Numerical Methods for Engineers, McGraw Hill International Edition.
2. M K Jain, S R K Iyengar and R K Jain, Numerical Methods for Scientific and Engineering Computation, Wiley Eastern.
3. S S Shastri, Introductory Methods of Numerical Analysis, Prentice Hall of India.
4. B. S. Grewal, Numerical Methods in Engineering & Science, Khanna Publishers.
5. W.J. DeCoursey, Statistics and Probability for Engineering Applications With Microsoft Excel , Newnes.
6. Montgomery, D.C. and Runger, G.C. Applied Statistics and Probability for Engineers, John Wiley & Sons, 2011.

(b) Open source software and website:

1. Students can refer to video lectures available on the websites including NPTEL lecture series.
2. Students can refer to the CDs available with some reference books for the solution of problems using software/spreadsheets. Students can develop their own programs/spreadsheets for the solution of problems.

Suggested Course Practical List:

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 with inbuilt solvers for chemical engineering application
10. . Solution of PDE with inbuilt solvers for chemical engineering application.

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