Gyanmanjari
Innovative University

Course Syllabus
Gyanmanjari Institute of Technology
Semester-1 (M.Tech)

Subject: Mathematical and Statistical Methods in Chemical Engineering -METCH11502

Type of course: Major (Core)

Prerequisite: Engineering Mathematics

Rationale: Courses addressing numerical analysis techniques are in greater demand as a result of the growing significance of numerical methods in many scientific and technical fields. This is because numerical approaches provide solutions to practical issues when Typical analytical techniques don't work. As a result, engineering education would be lacking without a sufficient grasp of numerical techniques. Data collection, presentation, analysis, and application for problem-solving, decision-making, and product and process design are all covered by statistics.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks					Total Marks
CI	T	P	C	Theory Marks		Practical Marks		CA	
				ESE	MSE	V	P	ALA	
4	0	2	5	60	30	10	20	30	150

Legends: CI-Classroom Instructions; T – Tutorial; P - Practical; C – Credit; ESE – End Semester Examination; MSE- Mid Semester Examination; CA - Continuous Assessment; ALA-Active Learning Activities.

Course Content:

Sr. No	Course content	Hrs	% Weightage
1	**Equation Forms in Process Modeling:** 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	12	20
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	12	20

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.	12	20
4	**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)	12	20
5	**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	12	20

Continuous Assessment:

Sr. No	Active Learning Activities	Marks
1	**Preparation of Multimedia Presentations on Mathematical and Statistical Concepts:** Students will prepare PowerPoint presentations that include videos, animations, pictures, and graphics to clearly explain theoretical topics such as numerical methods, regression analysis, optimization, and ODE/PDE solutions. Faculty will assign specific chapters or subtopics to groups so that the entire syllabus is covered. Presentations will be conducted in class and the final files submitted on the GMIU Web Portal.	10
2	**Statistical Data Analysis Project:** Students will perform a data analysis and curve fitting exercise using Microsoft Excel, Python, or MATLAB. They will apply linear and polynomial regression, analyze data accuracy, and interpret model parameters. The report of results and conclusions will be submitted through the GMIU Web Portal.	10
3	**Algorithm Development and Coding Practice:** Students will develop and execute algorithms for solving linear and non-linear algebraic equations and differential equations using software such as MATLAB, SCILAB, or Python. The developed codes and results will be compiled into a technical report and uploaded to the GMIU Web Portal.	10
	Total	30

Suggested Specification table with Marks (Theory): 60

Distribution of Theory Marks (Revised Bloom's Taxonomy)							
Level	Remembrance (R)	Understanding (U)	Application (A)	Analyze (N)	Evaluate (E)	Create (C)
Weightage	10%	17%	50%	14%	09%	00%

Note: This specification table shall be treated as a general guideline for students and teachers. The actual distribution of marks in the question paper may vary slightly from above table.

Course Outcome:

After learning the course, the students should be able to:	
CO1	Solve system of linear algebraic equations
CO2	Fit relationship between two data sets using linear, non-linear regression.
CO3	Calculate maxima/minima and functions
CO4	Design, simulate and optimise chemical engineering operations and processes.

List of Suggested Practical

Sr. No	Suggested Practical
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	Sample Preparation for TEM analysis (Bulk metal, Powder sample, Brittle material) Implementation of algorithm for solution of non-Linear Algebraic Equations

Instructional Method:

The course delivery method will depend upon the requirement of content and the needs of students. The teacher, in addition to conventional teaching methods by black board, may also use any tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.

From the content 10% topics are suggested for flipped mode instruction. Students will use supplementary resources such as online videos, NPTEL/SWAYAM videos, e-courses. The internal evaluation will be done on the basis of Active Learning Assignment.

Practical/Viva examination will be conducted at the end of semester for evaluation of performance of students in the laboratory.

Reference 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 Shastry, 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.