

GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL ENGINEERING (05)

CHEMICAL ENGINEERING MATHS

SUBJECT CODE: 2140505

B.E. 4th SEMESTER

Type of course: Mathematics in Chemical Engineering

Prerequisite: Engineering Mathematics

Rationale: In chemical engineering, problems arising in heat and mass transfer, fluid mechanics, chemical reaction engineering, thermodynamics, modeling and simulation, etc. involve linear algebra, nonlinear algebraic equations, ordinary differential equations, partial differential equations, etc. The numerical methods give the solution of applied problems when ordinary analytical methods fail. The increasing importance of numerical methods has led to enhanced demand for courses dealing with the techniques of numerical analysis. It is therefore clear training in engineering would be incomplete without an adequate understanding of numerical methods. The students should gain ability which enables them to select the appropriate numerical technique to solve a given engineering problem.

Teaching and Examination Scheme:

Teaching Scheme			Credits C	Examination Marks						Total Marks
L	T	P		Theory Marks			Practical Marks			
			ESE (E)	PA (M)		ESE (V)		PA (I)		
				PA	ALA	ESE	OEP			
3	2	0	5	70	20	10	30	0	20	150

Content:

Sr. No.	Content	Total Hrs	%Weightage
1	Approximations and Errors: Types of Errors, Significant figures, Accuracy of Numbers, Precision, Error Propagation, Applications in Chemical Engineering	4	7.5
2	Solution of Algebraic and Transcendental Equations: Basic Properties of Equations, Relations between Roots and Coefficients, Descartes Rule of Sign, Synthetic Division of a Polynomial by a Linear Expression, Bracketing Methods (Bisection, Secant, Method of False Position or Regula Falsi, etc.), Convergence of Iterative Methods, Newton-Raphson Method, Newton-Raphson Method for Non Linear Equations in Two Variables, Algorithms & Computer Programming for all these Methods in Applications of Chemical Engineering	10	18.5
3	Solution of Linear Equations: Mathematical Background, Matrix inversion, Gauss Elimination, Gauss-Jordan Method, Gauss-Seidel Iteration Method, Jacobi's Method, Gauss-Seidel Method, Eigen Value Problem, Algorithms & Computer Programming for all these Methods in Applications of Chemical Engineering	8	15
4	Curve Fitting Method of Least Squares, Fitting a Straight Line and a Polynomial, Fitting a Non-linear Function, Fitting Geometric and Exponential Curves, Fitting a Hyperbola, a Trigonometric Function, etc., Algorithms & Computer	5	9

	Programming of Curve Fitting Methods		
5	Finite Differences & Interpolation: Finite Differences: Forward, Backward and Divided Differences Table, Central Differences, Newton's Forward, Backward and Divided Differences Interpolation Formula, Interpolation Polynomials, Lagrange Interpolation Formula, Inverse Interpolation, Algorithms & Computer Programming for all these Methods in Applications of Chemical Engineering	5	9
6	Numerical Differentiation & Integration: Differentiation Formula based on Tabulator at Equal and Unequal Intervals, Newton-Cotes Integration Formulas, Trapezoidal Rule and Simpson's 1/3 and 3/8 Rule, Algorithms & Computer Programming for all these Methods in Applications of Chemical Engineering	8	15
7	Ordinary Differential Equations : Taylor's Series and Euler's Method, Modifications and Improvements in Euler's Method, Runge-Kutta 2 nd Order & 4 th Order Methods, Milne's Predictor-Corrector Methods, Boundary Value Problems, Algorithms & Computer Programming for all these Methods in Applications of Chemical Engineering	9	17
8	Partial Differential Equations: Parabolic, Hyperbolic, Elliptic (Explicit method-finite difference), Applications in Chemical Engineering	5	9

Suggested Specification table with Marks (Theory):

Distribution of Theory Marks				
R Level	U Level	A Level	N Level	E Level
7	21	35	7	0

Legends: R: Remembrance; U: Understanding; A: Application, N: Analyze and E: Evaluate and above Levels (Revised Bloom's Taxonomy)

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.

Reference Books:

1. S C Chapra and R P Canale, Numerical Methods for Engineers, McGraw Hill International Edition.
2. John H Mathews, Numerical Methods for mathematics & science, 2nd Edition, Prentice Hall.
3. Pushpavanam S, Mathematical Methods in Chemical Engineering, Prentice Hall of India.
4. N W Loney, Applied Mathematical Methods for Chemical Engineers, CRC Press.
5. R G Rice, D D Do, Applied Mathematics and Modeling for Chemical Engineers, Wiley.
6. A Varma, M Morbidelli, Mathematical Methods in Chemical Engineering, Oxford University Press.
7. V G Jenson, G V Jeffreys, Mathematical Methods in Chemical Engineering, Elsevier.
8. Mickley, Reid, Sherwood, Applied Mathematics in Chemical Engineering, Tata McGraw Hill.
9. S K Gupta, Numerical Methods for Engineers, New Academic Science.
10. M K Jain, S R K Iyengar and R K Jain, Numerical Methods for Scientific and Engineering Computation, Wiley Eastern.
11. S S Shastry, Introductory Methods of Numerical Analysis, Prentice Hall of India.
12. B S Grewal, Numerical Methods in Engineering & Science, Khanna Publishers.
13. Kenneth J Beers, Numerical methods for chemical engineering, Cambridge University Press.

Course Outcome:

After learning the course the students should be able to:

- Understand the basic algorithms for solution of and be able to solve non-linear equations.
- Understand the basic algorithms for solution of and be able to solve linear algebraic equations.
- Be proficient in manipulation of logarithmic, exponential, and other non-linear functions in order to linearize and to regress non-linear expressions.
- Understand the basic algorithms for fitting curves to data.
- Understand the basic algorithms for solution of and be able to solve numerical integration problems.
- Understand the basic algorithms for solution of and be able to solve problems in ordinary differential equations.
- Be familiar with a variety of numerical methods for solving partial differential equations.
- Be proficient in the use of programming language such as C or FORTRAN and use of software such as Excel Spreadsheets, Polymath, Matlab or Scilab, etc. to solve the types of problems listed above.
- Deal comfortably when encountering and solving the types of problems listed above.
- Be able to apply the techniques learnt in this subject to the solution of a comprehensive design problem.

List of Open Source Software/learning website:

- Students can refer to video lectures available on the websites including NPTEL lecture series. <http://nptel.iitm.ac.in>
- Students can refer to the CDs available with some reference books for the solution of problems using softwares/spreadsheets. Students can develop their own programs/spreadsheets for the solution of problems.

ACTIVE LEARNING ASSIGNMENTS: Preparation of power-point slides, which include videos, animations, pictures, graphics for better understanding theory and practical work – The faculty will allocate chapters/ parts of chapters to groups of students so that the entire syllabus to be covered. The power-point slides should be put up on the web-site of the College/ Institute, along with the names of the students of the group, the name of the faculty, Department and College on the first slide. The best three works should submit to GTU.