GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Master of Engineering

Level: PG

Branch: Computer Aided Process Design

Course / Subject Code: ME01072031

Course / Subject Name : Numerical Methods in Chemical Engineering

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

Prerequisite:	Basic knowledge of Mathematics at under graduate level.
Rationale:	The development of fast, efficient and expensive computers has significantly increased the range of engineering problems that can be solved reliably. Numerical methods use computers to solve complex engineering problems by step-wise, repeated and iterative methods, which would otherwise be tedious or unsolvable by hand calculations. This course offers an overview of numerical methods from Chemical Engineering perspective to solve the complex engineering problems.

Teaching and Examination Scheme:

			Total Credits	**Assessment Pattern and Marks**				**Total Marks**
				Theory		**Tutorial / Practical**		
L	**T**	**PR**	**C**	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.	**Interpretation of Engineering Data:** Classification of measurements, Types of Errors, Significant figures, Accuracy of Numbers, Precision, Error Propagation Variance and Distribution of Random Errors.	4	10
2.	**Solution of Non Linear Algebraic Equations:** Basic properties of equations, Bisection method, Method of False Position, Secant method, Mullers method, Newton- Raphson Method, Comparison of methods.	5	10
3.	**Solution of Linear Algebraic Equations:** Cramer's rule, Matrix inversion, Gauss Elimination, Gauss-Jordan	5	10

	Method,Gauss-Seidel Iteration Method, Factorization method, Ill-conditioned equations, Comparison of methods.		
4.	**Empirical Laws & Curve Fitting:** Method of Least Squares, Fitting of linear equation, Fitting of non-linear equation, Method of group averages, Method of moments.	4	10
5.	**Finite differences and Interpolation:** Forward, backward and central difference formula. Newtons forward and backward interpolation formula, Gauss's forward and backward interpolation formula, Lagranges interpolation formula, SplineInterpolation, Cubic Spline.	5	10
6	**Numerical Integration:** Newton-Cotes Integration Formulas, Trapezoidal Rule and Simpson's Rules,Gaussian integration.	4	10
7	**Ordinary Differential Equations :** Euler's Method, Modifications and Improvements in Euler's Method. Runge-Kutta Methods, Boundary Value Problems, Shooting method.	5	10
8	**Partial Differential Equations:** Solution of Parabolic, Hyperbolic, Elliptic equations, Solution of Laplace and Poissons equation.	4	10
9	**Introduction to Programming:** Analytic and algorithmic solutions **Excel Fundamentals:** Interface, Entering and formatting data, Entering and formatting formulas, Built-in functions, Performing logical tests using IFstatement. **Paython Fundamentals:** Interface, Representation of numbers, Variables andbasic data structure, Functions, Branching statements. **MATLAB fundamentals:** Interface, Script and Function files, One and two dimensional arrays, Branching statements.	9	20
	Total	**45**	**100**

Course Outcomes:

After Completion of the Course, Student will able to:

No.	Course Outcomes	
01	Explain the concept of error, precision, significant digits and propagation of error in purview of numerical methods.	**U**
02	Select appropriate numerical method to solve chemical engineering problems.	**N**
03	Solve problems by using appropriate numerical method.	**A**
04	Select appropriate computation tool to solve chemical engineering problems.	**A**

Suggested Specification Table with Marks (Theory):

Distribution of Theory Marks					
R Level	**U Level**	**A Level**	**N Level**	**E Level**	**C Level**
15	25	50	10	--	--

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

References/Suggested Learning Resources:

(a) Books:

1. Numerical Methods for Engineers, S C Chapra and R P Canale, McGraw Hill Publication.
2. Numerical Methods in Engineering & Science, B. S. Grewal, Khanna Publishers.
3. Advanced Engineering Mathematics, Erwin Kreyszig, Wiley Publication.
4. Applied Mathematics in Chemical Engineering, Mickley, Sherwood, Reed, McGraw Hill Publication.
5. Numerical Method for Engineers, Santosh Gupta, New Age International Publishers.
6. Python Programming and Numerical Methods: A Guide for Engineers and Sceintists, Qingkai Kong, TimmySiauw, Alexandre Bayen, Academic Press.
7. Engineering Computations: An Introduction using MATLAB and Excel, Joseph C. Musto, William E.Howard, Richard R. Williams. Mc-Graw Hill.

(b) Open-source software and website:

1. NPTEL lecture series.

List of Experiments: (Minimum 6 experiments need to be performed)

1. Roots of non-linear equations using hand calculation.
2. Roots of non-linear equations using computational tools.
3. Solution of simultaneous linear algebraic equations using hand calculation.
4. Solution of simultaneous linear algebraic equations using computational tools.
5. Curve fitting and interpolation using hand calculation.
6. Curve fitting and interpolation using computational tools.
7. Numerical integration using hand calculation

8. Numerical integration using computational tools.
9. Solutions of ordinary differential equations using hand calculation.
10. Solutions of ordinary differential equations using computational tools.

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