GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Bachelor of Engineering
Level: UG
Branch: Chemical Engineering
Subject Code : BE03005041
Subject Name : Numerical Methods in Chemical Engineering

w. e. f. Academic Year:	2024-25
Semester:	3
Category of the Course:	Basic Science Course

Prerequisite:	Basics of Mathematics
Rationale:	The main objective of course is to introduce numerical methods and computational techniques to solve chemical engineering problems. This will provide a background for applying these methods to industrial problems.

Course Outcomes:

Sr. No.	CO statement	Marks % weightage
CO-1	To demonstrate the concept of error, precision, significant digits and propagation of error in purview of numerical methods.	10
CO-2	To apply appropriate numerical method to solve chemical engineering problems.	10
CO-3	To apply the concept of numerical methods to solve linear and non-linear equation/s.	30
CO-4	To estimate parameters of linear and non-linear model equations using curve fitting and interpolation techniques	20
CO-5	To Solve problems related to integration, differentiation and ordinary differential equations using appropriate numerical method.	30

Teaching and Examination Scheme:

Teaching - Learning Scheme (in Hours per Semester)					Total Credits = TH/30	Assessment Pattern and Marks					Total Marks
						Theory		Tutorial / Practical			
L	T	P	PBL*	TH		ESE (E)	PA (M)	PA/ (I)	PBL (I)	ESE (V)	
45	0	15	60	120	04	70	30	20	30	0	150

Where L = Lecture, T= Tutorial, P= Practical, TW/SL = Term-Work / Self-Learning, TH = Total Hours, ESE = End-Semester Examination, PA = Progressive Assessment

*** Problem Based Learning (PBL) aims to accommodate learning beyond syllabus as per clause 9.4 of NBA manual.**

Content:

Sr. No.	Content	Total Hrs
1	Approximations and Errors: Types of Errors, Significant figures, Accuracy of Numbers, Precision, Error Propagation, Applications in Chemical Engineering	03
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	08
	Equations in Two Variables (Numericals based on application in chemical engineering)	
3	Solution of Linear Equations: Mathematical Background of Matrices and its operations, Matrix inversion, Gauss Elimination, Gauss-Jordan Method, Gauss-Seidel Iteration Method, Jacobi's Method, Gauss-Seidel Method, Eigen Value Problem (Numericals based on application in chemical engineering)	07
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 (Numericals based on application in chemical engineering)	07
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 (Numericals based on application in chemical engineering)	06
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 (Numericals based on application in chemical engineering)	06
7	Ordinary Differential Equations: Taylor's Series and Euler's Method, Modifications and Improvements in Euler's Method, Runge-Kutta 2nd Order & 4th Order Methods, Milne's Predictor-Corrector Methods, Boundary Value Problems (Numericals based on application in chemical engineering)	08

Suggested Specification table with Marks (Theory): (For BE only)

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
10	**20**	**30**	**10**	**0**	**0**

Legends: R: Remembrance; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create 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. Numerical Methods for Engineers by Steven C. Chapra and Raymond P. Canale, McGraw Hill Education India Private Limited, 7th Edition, 2016.
2. Introductory Methods of Numerical Analysis by S. S. Shastry, Prentice Hall India Learning Private Limited, 5th Edition, 2012.
3. Numerical Methods in Engineering & Science by B. S. Grewal, Khanna Publishers, 11th Edition, 2013.
4. Numerical Methods for Scientific and Engineering Computation by M. K. Jain, S. R. K. Iyengar, and R.K. Jain, New Age International Private Limited, 7th Edition, 2019.

List of Open Source Software/learning website:

- Reference to NPTEL lectures can be made for a better understanding regarding various numerical methods.

- **List of suggested activities for Problem Based Learning:**

Activity	No. of Hours	Total Hours Claimed	Evaluation Criteria
Assignments on Numerical Techniques (Methods like Newton-Raphson, Gauss-Seidel, Runge-Kutta, etc.)	Completing five assignments (3h each)	15	Evaluated based on assignment submission
Implementing Numerical methods in MS-Excel spreadsheet	Doing Two Spreadsheets based assignments (5h each)	10	Reviewed based on the implementation, results and presentation of results analysis

Activity	No. of Hours	Total Hours Claimed	Evaluation Criteria
Solving Problems & Coding using MATLAB, SCILAB or Python	Solving two coding-based assignments (5h each)	10	Reviewed based on Implementation, result accuracy and efficiency of coding solutions.
Technical Video Demonstration on concepts like error analysis, equation solving, interpolation, integration, differentiation, etc.	Watching video content and Preparing a report (5h)	05	Assessment based on understanding the content, report and presentation reflecting learning outcomes.
Literature Review and Concept Mapping: Review 3–5 research papers on numerical applications in chemical engineering; create a visual map of methodologies and findings	Literature reading: 5h Concept Map creation: 5h	10	Relevance of literature, clarity and technical quality of the concept map
Online Course (MOOC/NPTEL/SWAYAM/edX, etc.) on numerical methods or computational techniques in chemical engineering	Minimum course duration of 10 hours	10	Assessment through an examination at the end of the course. Certificate submission required
Experimental Data Analysis Using Numerical Methods (Processing real or simulated experimental data using numerical techniques)	Data collection and processing (5h) + Interpretation and report writing (5h)	10	Evaluated based on accuracy, technical depth, and insights derived from data analysis
Numerical Modelling and Simulation of Engineering Systems (Developing mathematical models and performing simulations for chemical processes)	Model formulation (5h) + Simulation and result analysis (5h)	10	Evaluated based on model accuracy, computational efficiency, and interpretation of results
Independent Course Project on Advanced Numerical Methods (Exploring Emerging Techniques) or **Applying Numerical Methods to Solve**	Literature review/Analysis/ Solution Development (15h) + Report writing	20	Evaluated based on originality, technical depth, research findings, solution and presentation

Activity	No. of Hours	Total Hours Claimed	Evaluation Criteria
Complex Industrial Problems	and preparation (5h)		
Producing Technical Videos related to the Subject Content	Content development (5h) + Video creation and uploading on the department/college website (5h)	10	Reviewed based on the quality and effectiveness of the video content
Develping Posters, Charts, or PowerPoint Presentations on Subject related Technical Topics	Designing and presenting visual content	10	Assessed based on creativity, clarity, and presentation skills

Guidelines for Faculty

- The activities listed above are **suggestive**, and faculty members have the flexibility to select and modify them as needed.
- The **total self-learning hours remain fixed at 60 hours**, ensuring comprehensive coverage of numerical methods in chemical engineering.
- Faculty can **adjust the distribution of hours** across different activities while maintaining a balanced learning approach.
- All records pertaining to the evaluation and assessment of self-learning activities must be properly maintained and preserved at the institute level. These records should be made available to the university upon request.
- Institutes are encouraged to utilize digital platforms, such as Microsoft Teams, for effective record-keeping and to ensure transparency in the evaluation and assessment of self-learning activities.

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