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SARVAJANIK UNIVERSITY

Sarvajanik College of Engineering and Technology
Surat.

Bachelor of Technology (B.Tech)

B.Tech. Semester IV (Chemical Engineering)

Subject Name:Numerical Methods in Chemical Engineering **Subject Code: BTAS-11404**

Type of course: BSC
Prerequisite: Reasonable understanding of Calculus, Differential equations and Linear algebra.
Rationale: The subject includes the numerical techniques applied in the domain of chemical engineering like in thermodynamics, fluid flow operations, mass and energy balance, heat and mass transfer, chemical reaction engineering.

Teaching and Examination Scheme:

TEACHING SCHEME				Theory Marks			Practical Marks		Total Marks
L	T	P	C	TEE	CA1	CA2	TEP	CA3	
3	0	2	4	60	25	15	30	20	150

CA1: Continuous Assessment (assignments/projects/open book tests/closed book tests **CA2:** Sincerity in attending classes/class tests/ timely submissions of assignments/self-learning attitude/solving advanced problems **TEE:** Term End Examination **TEP:** Term End Practical Exam (Performance and viva on practical skills learned in course) **CA3:** Regular submission of Lab work/Quality of work submitted/Active participation in lab sessions/viva on practical skills learned in course

Content:

Sr. No.	Content	Total Hours	% Weightage
01	**Solution of Algebraic and Transcendental Equations:** Basic Properties of Equations, Bracketing Methods [Bisection, False Position]and open methods [Newton Raphason Method, iterative Method, Secant Method] **Applications:**Defining and solving equations for steady and dynamic flow systems, cubic equations of state, Roult's Law, VLE, Colebrook equation and bubble/dew point temperature for binary mixture.	06	15%
02	**Solution of Linear Equations:** Mathematical Background, Direct and iterative methods such as matrix inversion, Gauss-elimination, Gauss-Jordan, Jacobi and Gauss-Seidal method. **Applications:**Defining and solving linear equations for mass balance for reactors, heat and mass transfer operations.	06	10%
03	**Curve Fitting:** Fitting a Straight Line and a Polynomial, Fitting a Non-linear Function, Fitting Geometric and Exponential Curves, **Applications:** Discrete data analysis for various chemical processes and operations by using Method of Least Squares,	08	20%
04	**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.	08	20%

	Applications: Study of temperature, pressure and composition effects on properties of substances, Chemical Kinetics and FT-IR.		
05	**Numerical Differentiation & Integration**: Newton-Cotes Integration Formulas, Trapezoidal Rule and Simpson's 1/3 and 3/8 Rule. Applications:Formulation of problem and solution of differential equations for Velocity of fluids in a pipe, Different Chemical kinetic models & RTD analysis of Reactors, heat, mass & momentum balance for various chemical engineering systems	05	10%
06	**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, **Applications:**Defining a problem with Chemical Engineering aspects such as flow through tank, linear second order dynamic systems, reaction kinetics.	12	25%

Suggested Specification table with Marks (Theory& Practical):

Distribution of Theory Marks					
R Level	**U Level**	**A Level**	**N Level**	**E Level**	**C Level**
20	**25**	**25**	**20**	**10**	**0**

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

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

Reference Books:

Sr no	Title of book /article	Author(s)	Publisher and details like ISBN	Year of publication	Publication Edition
1.	Numerical Methods for Engineers	S.C. Chapra and R. P. Canale	Tata McGraw Hill		International edition
2.	Numerical Methods in Engineering and Science	B. S. Grewal	Mercury Learning and Information(2019)/ Khanna Publisher (3rd Edition, 2014)	2019	3rd Edition
3.	Numerical Methods in Chemical Engineering	PradeepAhuja	PHI		1st Edition
4.	Numerical Methods for Chemical Engineers using Excel, VBA and MATLAB.	Victor J. Law	CRC Press	2013	1st Edition,
5.	Applied Mathematical Methods in Chemical Engineering	N W Loney	CRC Press	2015	3rd Edition,
6.	Advanced Engineering Mathematics	Erwin Kreyszig	Jhon Wiley and Sons		10th Edition

7.	Advanced Engineering Mathematics	S. R. K. Iyengar, R. K. Jain.	Narosa Publishing		5th Edition
8.	Elements of Applied Mathematics. Volume 1	P.N.Wartikar and J.N.Wartikar, Pune VidyarthiGraha	McGraw Hill Kogakusha Co.		2nd Edition
9.	Introductory Methods of Numerical Analysis	S. S. Sastry	PHI		5th Edition
10.	Numerical Solution of differential Equations	M. K. Jain	Wiley Eastern		4th Edition
11.	Stoichiometry: Material and Energy Balance Computations	Bhatt B. I., Thakore S.B., Shah S.R.	Tata McGraw Hill Company	2021	6th Edition

Course Outcome:

Sr. No.	After learning this subject, students will be able to	Weightage in %
CO-1	Students should be able to solve system of linear algebraic and non-linear equations.	20
CO-2	Students should be able to do numerical integrations of functions.	15
CO-3	Students should be able to fit relationship between two data sets using linear, non-linear regression.	10
CO-4	Students should be able to solve simple first and second order ODE and PDE by numerical methods.	35
CO-5	Students will be able to solve analyse the data and predict the behaviour of process variable based on probabilistic data.	20

Mapping with POs:

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PO 12	PSO 1	PSO 2	PSO 3
CO-1	2	2	2	2	2	2	2	3	3	2	3	3	3	2	3
CO-2	2	3	2	2	3	2	2	3	3	2	3	3	3	2	3
CO-3	3	3	2	2	2	3	3	3	3	2	3	3	3	3	3
CO-4	3	3	1	2	2	3	3	3	3	2	3	3	3	3	3
CO-5	3	3	2	1	2	3	3	3	3	2	3	3	3	3	2
Rationale*	13	14	9	9	11	13	13	15	15	10	15	15	15	13	14

Rationale*: Explaining why it is matching this particular program outcome

List of Open learning website:NPTEL lectures. Simulation software SCLAB learning version is available free online.

List of Open Source Software:SCILAB, R

LIST OF PRACTICALS

Following set of systems is to be solved using softwares e.g. SCILAB, MS Excel etc.

1. Solution of Non-linear equations using Bisection, False position, Secant, Newton-Raphson method.
2. Solution of Simultaneous linear equations using Gauss-elimination, gauss-Jorden, Matrix inversion, Jacobi and Gauss-seidel Methods.
3. Curve fitting using least square method.
4. Interpolation using Newton's forward/backward, Gauss forward/backward, Langranges, Newton's divided difference method.
5. Numerical integration using trapezoidal rule, simpson's 1/3 and 3/8 method.
6. Solution of ordinary differential equation using Euler's and modified Euler's method, R-K 2nd order and 4th order method, Milne's predictor-corrector method and finite difference method.

Major Equipment: Computer Lab