

**Subject Code: 01MA0401**

**Subject Name: Numerical Methods in Chemical Engineering**

**B.Tech. Year: II (Semester IV)**

**Objective:** To impart knowledge of solving the mathematical problems related to chemical engineering by using numerical methods.

**Credits Earned:** 4 Credits

**Course Outcomes:** After completion of this course, student will be able to:

1. Understand the basic concepts of numerical methods.
2. Apply the concept of Interpolation on various data set.
3. Solve the algebraic equations and numerical integration problems using numerical methods.
4. Solve the ordinary and partial differential equation using best suitable numerical techniques.

**Pre-requisite of course:** None

**Teaching and Examination Scheme**

Teaching Scheme (Hours)			Credits	Theory Marks			Tutorial/ Practical Marks		Total Marks
Theory	Tutorial	Practical		ESE (E)	IA (I)	CSE (C)	Viva (V)	Term work (TW)	
3	1	0	4	50	30	20	25	25	150

**Contents:**

Unit	Topics	Contact Hours
1	<b>Solution of Equations and Numerical Integration</b> Finding the roots of a transcendental and algebraic equation, Direct and Indirect methods, Bisection method, Regula-Falsi method, Newton-Raphson method. Solution for Simultaneous linear system of equations: Gauss Jacobi method, Gauss-Siedel method. Overview of non-linear system of equation	<b>10</b>
2	<b>Interpolation</b> Finite difference, Forward and backward differences, Interpolation and Extrapolation, Newton's forward interpolation, Newton's backward interpolation. Lagrange's interpolation, and Newton's divided difference	<b>8</b>



	interpolation.	
3	<b>Numerical Integration</b> Introduction to numerical methods, Trapezoid method, Simpson's 1/3rd rule, Simpson's 3/8th rule, Gaussian one point, two-point, three-point quadrature.	<b>8</b>
4	<b>Ordinary and Partial Differential Equations</b> Numerical solution to Ordinary differential equation: Taylor's Series and Euler's Method, Predictor-corrector technique, Runge-Kutta methods, Boundary Value Problems. Numerical solution to elliptic, parabolic and hyperbolic partial differential equations.	<b>12</b>
	<b>Total Hours</b>	<b>38</b>

**List of Tutorials (Using Excel/MATLAB/or any other computational tool):**

1. Tutorial forward and backward differences.
2. Tutorial on Bisection method.
3. Tutorial on Linear and Non-Linear curve fitting on given data set.
4. Tutorial on Regula-Falsi method
5. Tutorial on Polynomial root finding techniques: Newton Raphson's Method.
6. Tutorial on numerical integration: Trapezoidal rule and Simpson 1/3 rule.
7. Numerical on forward and backward difference interpolation.
8. Tutorial on Lagrange's and Newton's divided difference interpolation.
9. Tutorial on Euler's Method for solving ordinary differential equations.
10. Tutorial on solving ODE by Runge-Kuttamethod.

**References:**

1. "Miller and Freund's Probability and Statistics for Engineers", Richard A Johnson, Prentice Hall of India, 2011.
2. "Introductory Methods of Numerical Analysis", S.S. Sastry, Prentice Hall of India, 2012.
3. "Numerical Methods For Engineers", Santosh K. Gupta, New Age Intl. Publishers, New Delhi, 2010.
4. "Numerical Methods for Engineers" S. C. Chapra and R. P. Canale, 5th Ed., McGraw Hill, 2006.
5. "Numerical Methods in Engineering & Science", B S Grewal, Khanna Publishers, 1996.



**Suggested Theory distribution:**

The suggested theory distribution as per Bloom's taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery and evaluation					
Remember	Understand	Apply	Analyze	Evaluate	Create
20%	20%	30%	20%	10%	-

**Instructional Method:**

- The course delivery method will depend upon the requirement of content and need of students. The teacher in addition to conventional teaching method by black board, may also use any of tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.
- The internal evaluation will be done on the basis of continuous evaluation of students in the laboratory and class-room.
- Practical examination will be conducted at the end of semester for evaluation of performance of students in laboratory.
- Students will use supplementary resources such as online videos, NPTEL videos, e-courses, Virtual Laboratory

**Design Based Problems (DP)/ Open Ended project (OEP) :**

In the beginning of the session, subject faculty will allot an OEP / DP to the students. Students will be free to choose a topic of their choice which will be relevant to the syllabus and they will either prepare a working model/ report / presentation / poster on their topic.

**Web Resources:**

- <https://nptel.ac.in/courses/103106112>
- <https://nptel.ac.in/courses/103106118>
- <http://numericalmethods.eng.usf.edu>