LOK JAGRUTI UNIVERSITY (LJU)

INSTITUTE OF ENGINEERING AND TECHNOLOGY

Department of Chemical Engineering (708)

Bachelor of Engineering (B.E.) -Semester–IV

Course Code:	**017083405**
Course Name:	**Numerical Methods in Chemical Engineering**
Category of Course:	Professional Core Course (PCC)
Prerequisite Course:	None

Teaching Scheme				
Lecture (L)	**Tutorial (T)**	**Practical (P)**	**Credit**	**Total Hours**
4	**1**	**0**	**5**	**50**

Syllabus

Unit No.	Topic	Prerequisite Topic	Successive Topic	Teaching Hours
01	**Approximations and Errors in Computation**			**2 (4%)**
	1.1 Accuracy of numbers	---	---	
	1.2 Precision	---	---	
	1.3Types of errors	---	Introduction to Industrial Instrumentation(017083504-Unit-7)	
	1.4Error propagation	---	Introduction to Industrial Instrumentation(017083504-Unit-7)	
02	**Solution of Algebraic and Transcendental equations**			**6 (12%)**
	2.1 Bracketing and Open methods(Iterative methods)	Basic Algebra(017081191-Unit-1)	---	
	2.2 Bisection method	---	---	
	2.3 Newton Raphson method	---	---	
	2.4 Secant method	---	---	
	2.5 Regula Falsi method(Method of False Position or Regula-Falsi Method or Interpolation Method)	---	---	
	2.6 Applications in Chemical Engineering	---	---	
03	**Solution of simultaneous algebraic equations**			**5 (10%)**
	3.1 Direct method to solve linear simultaneous equations–Gauss Elimination, Gauss Jordan method	---	---	
	3.2Iterative methods-Gauss Jacobi and Gauss Seidel method	---	---	
	3.3Comparison between various methods	---	---	
04	**Curve Fitting**			**5 (10%)**
	4.1 Method of Least squares	Sequence and Series(017081191-Unit-4)	---	
	4.2 Fitting of straight line and quadratic curve(working procedure)	---	---	
	4.3 Fitting of exponential curve	---	---	
	4.4 Fitting of Geometric curve	---	---	
	4.5 Applications in Chemical Engineering	---	---	
05	**Finite differences and Interpolation**			**7 (14%)**
	5.1 Finite differences(Forward differences, Backward differences)	---	---	
	5.2 Operators and relation between the operators	---	---	
	5.3 Newton’s forward and backward Interpolation	---	---	
	5.4 Lagrange’s Interpolation	---	---	
	5.5 Newton’s Divided Difference Interpolation	---	---	
	5.6Applications in Chemical Engineering	---	---	
06	**Numerical Differentiation and Integration**			**5 (10%)**
	6.1 Numerical Differentiation(Derivates using Newton’s forward difference formula, Derivates using Newton’s backward difference formula)	Basic Differentiation and Integration-(017081191-Unit-3)	Linear Open Loop System (017083504	
	6.2 Trapezoidal rule	Basic Differentiation and Integration-(017081191-Unit-3)	Linear Open Loop System (017083504	
	6.3 Simpson’s $1/3^{rd}$ rule	Basic Differentiation and Integration-(017081191-Unit-3)	Linear Open Loop System (017083504	
	6.4 Simpson’s $3/8^{th}$ rule	Basic Differentiation and Integration-(017081191-Unit-3)	Linear Open Loop System (017083504-Unit-2)	
07	**Solution of Ordinary differential equation**			**4 (8%)**
	7.1 Taylor’s series method	Solution of simultaneous equations(ODE)(01708129	---	

		1-Unit-7)		
	7.2Euler's and Modified Euler's method	Partial Derivatives(017081191-Unit-5)	---	
	7.3 RungeKutta 2nd and 4th order method	---	---	
08	**Solution of Partial differential equation**			**4 (8%)**
	8.1 Classification of Second order equations	Partial Derivatives(017081191-Unit-5)	Linear Open Loop System (017083504-Unit-2)	
	8.2 Solution of Laplace equation	Partial Derivatives(017081191-Unit-5)	Linear Open Loop System (017083504	
	8.3 Solution of Poisson's equation	Partial Derivatives(017081191-Unit-5)	Linear Open Loop System (017083504	
09	**Optimization techniques**			**6 (12%)**
	9.1 One dimensional unconstrained optimization	---	---	
	9.2 Multidimensional unconstrained optimization	Basic Differentiation and Integration-(017081191-Unit-3)	---	
	9.3 Constrained optimization	Basic Algebra(017081191-Unit-1)	---	
10	**Linear Programming**			**6 (12%)**
	10.1 Graphical method	Basic Algebra(017081191-Unit-1)	---	
	10.2 Simplex method	---	---	

Proposed Theory + Practical Evaluation Scheme by Academicians (% Weightage Category Wise and it's Marks Distribution)					
L:	**4**	**T:**	**1**	**P:**	**0**
Note: In Theory Group, Total 4 Test (T1+T2+T3+T4) will be conducted for each subject. Each Test will be of 25 Marks. Each Test Syllabus Weightage: Range should be 20% - 30%					
Group (Theory or Practical)	**Group (Theory or Practical) Credit**	**Total Subject Credit**	**Category**	**% Weightage**	**Marks Weightage**
Theory	**5**	**5**	MCQ	10%	20
Theory			Theory Descriptive	10%	10
Theory			Formulas and Derivation	20%	10
Theory			Numerical	60%	60
Expected Theory %	**100%**		**Calculated Theory %**	**100%**	**100**
Practical	**0**		Individual Project	0%	0
Practical			Group Project	0%	0
Practical			Internal Practical Evaluation (IPE)	0%	0
Practical			Viva	0%	0
Practical			Seminar	0%	0
Expected Practical %	**0%**		**Calculated Practical %**	**0%**	**0**
Overall %	**100%**			**100%**	**100**

Course Outcome	
	Upon completion of the course students will be able to
1	Develop comprehensive knowledge of numerical computation accuracy, error management, and propagation, alongside mastering diverse algebraic and transcendental equation-solving techniques
2	To utilize the Method of Least Squares for curve fitting across various curve types, and comprehend its application in problem-solving, alongside mastering finite differences and interpolation techniques and their relevance in Chemical Engineering applications.
3	Gain proficiency in numerical techniques for differentiation and integration, as well as solving ordinary and partial differential equations for engineering problem-solving.
4	To apply optimization techniques, including unconstrained and constrained methods, along with linear programming approaches such as the graphical and simplex methods.
Suggested Reference Books	
1	"Numerical Methods in Engineering and Science", Dr B S Grewal, Khanna Publishers, August 2014.
2	"Numerical Methods for Engineers", S C Chapra and R P Canale, McGraw Hill International Edition.
3	"Numerical Methods for Scientific and Engineering Computation", M K Jain, S R K Iyengar and R K Jain ,Wiley Eastern.

List of Open-source Software/Learning Website	
1	https://nptel.ac.in/