Course Type	Course Code	Name of Course	L	T	P	Credit
DC	NCHC503	Computational Techniques in Chemical Engineering	3	1	0	4

Course Objective
• To lay a solid foundation for introductory and advanced computational techniques that are relevant in solving a wide variety of chemical engineering problems. • Essentially, it is an advanced numerical analysis course at the postgraduate level that stresses on understanding the various numerical schemes, and a comparative assessment of the various advantages and limitations of such schemes.
Learning Outcomes
The students will • be proficient in solving chemical engineering problems using computational techniques and tools. • be able to make an informed choice regarding selecting/discarding a particular numerical scheme while attempting to solve a problem numerically. • develop a solid and fundamental understanding of numerical methods, that is indispensable towards writing in-house codes, or employing commercial numerical solvers for solving an engineering problem of interest.

Unit No.	Description of Lectures	Class Hours	Learning Outcomes
1.	**Introduction to computational tools and techniques:** Motivation for adopting numerical techniques towards solving problems in science and engineering; Error analysis: Truncation and round-off errors, representation of errors, accuracy and precision.	2 L + 0 T	Students will understand the diverse application of computational methods, and will get acquainted with the basics of error estimation and analysis.
2.	**Numerical approach to obtaining roots of single-variable equation and multivariable equations:** Classification of root-finding methods (open and bracketing methods); Study of different open and bracketing methods like bisection, regula-falsi, successive substitution, Newton-Raphson, secant; Different methods for solving polynomial equations like Horner's method, Müller's method; Multivariable Newton-Raphson method	5 L + 2 T	Students will learn to solve algebraic and transcendental non-linear equation(s) using a number of numerical schemes. They will also comprehend the advantages and limitations of each of these methods.
3.	**Numerical solution of system of linear algebraic equations:** Gauss elimination; Gauss-Jordan; Gauss-Siedel; LU decomposition; Cholesky decomposition; QR factorisation, Tridiagonal matrix algorithm approaches	5 L + 3 T	Students will learn to solve system of linear equations, especially sparse systems using computationally efficient algorithms.

4.	**Numerical optimisation:** Unconstrained optimisation: single- and multi-dimensional; Constrained optimisation	**5 L + 2 T**	Students will learn the basics of optimization, and their application towards solving diverse range of chemical engineering problems.
5.	**Regression and Interpolation:** Linear and non-linear regression analysis; Newton's forward, backward and divided interpolation; Lagrange's interpolation; Spline interpolation; orthogonal polynomials	**6 L + 2 T**	Students will get acquainted with regression and interpolation in order to model datasets.
6.	**Numerical solution of ordinary differential equations (ODEs):** Types of ODEs; Initial value problems: Euler and Runge-Kutta methods; collocation methods; System of ODEs and adaptive Runge-Kutta methods; Boundary value problems: shooting and finite difference methods; stiff ODEs, stability and convergence in ODEs; solution of differential algebraic systems (DAEs)	**9 L + 3 T**	Students will get exposed to a diverse range of linear and non-linear ODEs arising in chemical engineering, and specialized techniques to solve them depending on their stiffness
7.	**Numerical solution of partial differential equations (PDEs):** Classification of second order linear PDEs; Use of various finite difference-based algorithms to solve elliptic and parabolic PDEs arising in chemical engineering; introduction to finite element methods	**10 L + 2 T**	Students will learn the basics of PDEs, and how to solve parabolic and elliptic PDEs using finite difference and finite element schemes.
	Total	**56**	

Textbooks:

1. Steven C. Chapra and Raymond P. Canale (2021), Numerical Methods for Engineers 8th ed., McGraw Hill.

2. Joe D. Hoffman (2001), Numerical Methods for Engineers and Scientists 2nd ed., CRC Press.

Reference books:

1. William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery (2007), Numerical Recipes: The Art of Scientific Computing 3rd ed., Cambridge University Press.

2. Santosh K. Gupta (2019), Numerical Methods for Engineers 4th ed., New Age International Publishers.

3. Mark E. Davis (2013), Numerical Methods and Modelling for Chemical Engineers, Dover Publications.

4. Alkis Constantinides and Navid Mostoufi (1999), Numerical Methods fort Chemical Engineers with MATLAB Applications, Prentice Hall.