Course Type	Course Code	Name of Course	L	T	P	Credits
DP	NCHC504	**Computational Techniques Lab**	0	0	3	1.5

Course Objective

- To complement the theory course on Computational Techniques in Chemical Engineering, and provide the students a hands-on experience regarding writing computer codes (in MATLAB) for solving a wide range of chemical engineering problems

Learning Outcomes

- The students will be proficient in writing codes in MATLAB from scratch, implementing the various numerical algorithms that they are learning in the theory course on Computational Techniques in Chemical Engineering.
- By the end of this course, they will have a repository of codes with themselves, which can be suitably employed later on to solve more computationally-intensive engineering problems in future.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1.	Introduction to MATLAB, and its utility towards solving computational problems encountered in chemical engineering . Developing a computer program for the numerical solution of single and multivariable non-linear algebraic equation using: (a) Bisection method, (b) Regula-falsi (c) Newton-Raphson method	6	Learners will become familiar with MATLAB, and have understanding of root-finding methods.
2.	Developing a computer codes for the numerical solution of system of simultaneous linear algebraic equations : a) Gauss elimination method, b) Gauss Seidel iterative method c) LU decomposition, d) Thomas algorithm	6	Learners will implement the various numerical methods for solving system of linear equations
3.	Linear and non-linear regression using data relevant for chemical engineering	6	Learners will understand the role of trend analysis for a given set of data
4.	Developing a computer program to perform different kinds of interpolation (Newton's forward, backward, and divided differences; Lagrange's interpolation; spline interpolation)	6	Learners will be able to write a code to interpolate in cases where precise dataset is available

5.	Developing a computer program for the numerical solution of a set of ordinary differential equations (both IVP and BVP) using a) Euler method (b) 4^{th} order Runge-Kutta method, c) higher order predictor-corrector methods d) shooting method, e) finite difference method	12	Learners will get acquainted with the various numerical techniques meant for solving ODEs, and their implementation via writing robust code
6.	Developing a computer program for the numerical solution of elliptic partial differential equations: Liebmann method	3	Learners will get proficient in solving steady-state multidimensional chemical engineering problems
7.	Developing a computer program for the numerical solution of parabolic partial differential equations: Crank-Nicholson method	3	Learners will get proficient in solving unsteady state chemical engineering problems using higher-order accurate methods
	Total Contact hours:	**42**	

Text Books:

1. Steven C. Chapra (2019),*Applied Numerical Methods with MATLAB for Engineers and Scientists 4th Ed.*, McGraw Hill.

Reference Books:

1. S. Attaway (2022), *MATLAB: A Practical Introduction to Programming and Problem Solving, 6th Ed.*, Butterworth-Heinemann.
2. 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.
3. Santosh K. Gupta (2019), *Numerical Methods for Engineers 4th ed.*, New Age International Publishers.
4. Mark E. Davis (2013), *Numerical Methods and Modelling for Chemical Engineers*, Dover Publications.