PCH201 COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING

L	T	P	Cr
3	0	2	4

Course Objective:
To learn various computational techniques for analysing and solving chemical engineering problems.

Solution of Algebraic Equations: Solution of non-linear and transcendental equations in one or more than one variable, Solution of linear simultaneous equations, Solution of equations by computer programming, Excel sheet, Poly Math, and MATLAB.

Solution of Ordinary Differential Equations: Initial value problem: RK class and predictor corrector class methods, stiff ODE's and Gear's methods, Boundary value problem: Shooting methods, finite difference method, method of weighted residuals and orthogonal collocation and Galerkin technique to solve BVP in ODEs, Solution of Chemical Engineering problems (ODEs) by computer programming, excel sheet, Poly Math, and MATLAB.

Solution of Partial Differential Equations: Classification of PDEs: Parabolic, elliptical and hyperbolic equation, Review of finite difference techniques to solve partial differential equation, Application to chemical engineering systems, Concept of finite element, Similarity transformation, Method of weighted residuals, Orthogonal collocation, Least square, Finite element methods to solve PDEs with application to Chemical Engineering systems using MATLAB.

Course learning outcomes (CLOs):

The students will be able to

1. solve problems of algebraic and differential equations, simultaneous equation, partial differential equations
2. convert problem solving strategies to procedural algorithms and to write program structures
3. solve engineering problems using computational techniques
4. assess reasonableness of solutions, and select appropriate levels of solution sophistication

Recommended Books:

1. *Gerald, C.F., and Wheatley P. O., Applied Numerical Analysis, Pearson Education (2006).*
2. *Finlayson, B.A., Introduction to Chemical Engineering Computing, Wiley Interscience (2012).*
3. *Beers, K.J., Numerical Methods for Chemical Engineering, Applications in MATLAB, Cambridge University Press (2007).*

Evaluation Scheme:

S.No.	Evaluation Elements	Weightage (%)
1.	MST	25
2.	EST	40
3.	Sessional (may include Assignments/Projects/Tutorials/Quizes/Lab Evaluations)	35