Computations Lab for Chemical Engineering Applications

Course Code: 22CH1113

L	T	P	C
0	0	3	1.5

Course Outcomes: At the end of the course the student shall be able to
CO1: Using python nonlinear algebraic and transcendental equations using numerical methods (L2)
CO2: Apply curve fitting techniques to approximate a function in interpolating and extrapolating a given data. (L3)
CO3: Solve ordinary differential equations by Euler's method and Runge Kutta method. (L3)
CO4: Apply numerical methods to boundary value problems and partial differential equations. (L3)
CO5: Apply finite difference schemes to solve partial differential equations. (L3)

Introduction

Basic calculations like matrix manipulations, calculating eigen-values and eigen- vectors.
Roots of polynomials.
Basic plotting: Putting texts and legends, Labeling axes, Multiple plots, phase plots, semi-log and log-log plots.

List of Experiments

Polynomial and non-linear regression:

1. Given Cp vs T data, calculate the constants in specific heat equation
2. Given P, V and T values, calculate the constants in a cubic EOS.
3. Given T, x and y values, calculate the two constants in Margules equation and Van Laar equation.
4. Parameter estimation and Non-linear Regression.

Non-linear algebraic equations:

5. Friction factor in turbulent flow.
6. Bubble point and Dew point calculations for ideal and non-ideal solutions.
7. Calculating Activity coefficient parameters with VLE data.
8. e1, e2 calculations in two equilibrium reactions.

Ordinary Differential equation (IVP): (Using Runge-Kutta method (RK)

9. Gravity flow tank.
10. Absorber column.
11. Two Tank coupled system.

Ordinary Boundary Value problem (BVP): Drichlet, Robin & Neumann boundary conditions using finite difference scheme

12. heat transfer in a slab, heat transfer in a fin or analogous equations Partial Differential equations:
13. One dimensional unsteady heat conduction problem (and similar equations) by finite differencing in space and integrating in time using RK method for different boundary conditions.
14. Heat Transfer in composite walls.