

## CH455: PROCESS MODELING, SIMULATION & OPTIMIZATION

CREDITS = 6 (L = 4, T=0, P = 2)

1. **MODELING:** Fundamentals of mathematical models, principles of formulation, lumped and distributed parameters models- hydraulic tank, mixing vessel, simultaneous mass and energy balance, continuous stirred tank heater and reactor, batch reactor, reactor with mass transfer, heat exchanger, single component vaporizer, multi-component flash drum, ideal binary distillation column. 14 Hours
2. **OPTIMIZATION:** Basic concepts; one variable optimization (Newton's method, Secant methods, dichotomous search, Fibonacci, golden section method); two or more variables (direct, indirect, Secant methods and linear programming). 20 Hours
3. **SIMULATION:** Continuous and dynamic simulation (packages and languages), techniques of digital simulation, developing description of information flow, process to information flow diagram and information flow diagram to numerical form, idea of computer aided design, digital simulation of continuous stirred tank reactor, binary distillation column. Flowsheeting and flowsheeting codes. Equation and modular based flowsheeting. 6 Hours

### REFERENCE BOOKS

Title: Process Modeling, Simulation and Control for Chemical Engineers  
Author: W.L. Luyben  
Publisher: Mc Graw Hill

Title: Optimization of Chemical Process  
Author: Edgar and Himmelblau  
Publisher: McGraw-Hill International edition

Title: Chemical Process Simulation  
Author: Asghar Hussain  
Publisher: Wiley Eastern Ltd., New Delhi.

Title: Modeling and Simulation in Chemical Engineering  
Author: Roger G. Frank  
Publisher: Wiley Inter Science, New York

## ***LIST OF EXPERIMENTS***

- 1**            *Introduction to MATLAB*
- 2.**        Introduction to MATLAB
- 3.**        Write a program to add, subtract, multiply or divide two numbers or vector or matrix
- 4.**        Introduction of Design II
- 5.**        Introduction of HTRI
- 6.**        Root Finding method (Single Variable):  
            Quasi Newton method/ Newton Raphson Method
- 7.**        Root Finding method (Single Variable):  
            Using fsolve, fzero
- 8.**        Optimization techniques:  
            Fibonacci/ Equal Interval method
- 9.**        Optimization techniques:  
            Newton Raphson/Quasi Newton Raphson
- 10.**      Simulation of system of Linear Equations
- 11.**      Simulation of System of Non-Linear Equations
- 12.**      Introduction of ODE solver
- 13.**      Simulation of System of ODEs using built in solver
- 14.**      Simulation of System of ODEs using Euler and Runge-Kutta 4<sup>th</sup> order methods
- 15.**      Parameter Estimation
- 16.**      Linear Programming Problem