

# AMCH23 PROCESS SIMULATION & DESIGN

## UNIT-1 GENERAL CONCEPT OF SIMULATION / DESIGN

- 1.1 Introduction to models,
- 1.2 Design problem vs Simulation Problem
- 1.3 Approaches to simulation
- 1.4 A brief outline of components of a CAD package in Chemical Engineering
- 1.5 Thermodynamic and physical property package,
- 1.6 Module library, numerical routines library, costing etc.

## UNIT-2 MATHEMATICAL MODELS, MODEL BUILDING, PARAMETER ESTIMATION

- 2.1 Mathematical Models, their classification (deterministic vs stochastic, linear vs non-linear, lumped parameter vs distributed parameter, dynamic vs steady-state with examples)
- 2.2 Model building (writing down equations only) examples
  - (i) homogenous well mixed and plug flow reactor (isothermal and non-isothermal)
  - (ii) heated tank
  - (iii) flash drum
  - (iv) gas-liquid bubble reactor
  - (v) Countercurrent multistage liquid extraction
- 2.3 Parameter Estimation by Least square (linear and quadratic)

## UNIT-3 NON-LINEAR

- 3.1 Solution to systems of non-linear algebraic equations (Newton's and Successive substitution)
- 3.2 Application in Chemical engg. such as equilibrium flash calculations equations of state, reaction equilibrium etc

## UNIT-4 ODE

- 4.1 Solutions of single ODE and systems of ODEs (Implicit Euler & Runge- Kutta IV th Order)
- 4.2 Applications to chemical engineering problems such as homogenous well mixed reactor (isothermal and non-isothermal) and heated tank.
- 4.3 Models of difference equations Applications to chemical engineering – Counter-current multistage liquid extraction

## UNIT-6 SIMULATION OF SINGLE UNITS

- 6.1 Simulation of single units (modules)
- 6.2 Degree of freedom (with and without system constraints)
- 6.3 Coupling and Decoupling of equations
- 6.4 Precedence ordering for Design / Simulation (partitioning and tearing)
- 6.5 Selection of design variable algorithm and persistent recycles

## UNIT-7 SIMULATION OF COMPLETE FLOW SHEET

- 7.1 Simulation of complete flow sheet

7.2 Degrees of freedom for flow sheet with connecting equations

7.3 Approaches to simulation:

(I) Sequential modular

A) Precedence ordering of Modules (Partitioning and Tearing of flow sheets)

(II) Simultaneous

A) Equation solving

B) Simultaneous Modular with linearized modules

## **UNIT-8 BATCH PROCESS SIMULATION BATCH DISTILLATION BATCH REACTORS**

### **Reference Books:**

1. Chemical Plant Simulation by Crowe C M
2. Process Flow sheeting by Westerberg A W

