

# Modeling & Simulation in Chemical Engineering

B.E. Sem. VIII [CHEM]

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## EVALUATION SYSTEM

	Time	Marks
<b>Theory Exam</b>	3 Hrs.	100
<b>Practical &amp; Oral</b>	–	25
<b>Oral Exam</b>	–	–
<b>Term Work</b>	–	25

## SYLLABUS

### 1. Mathematical Models of Chemical Engineering System

Introduction, Uses of Mathematical Model, Scope of Coverage, Principles of Formulation, Fundamental Laws, Mathematical models, their classification (deterministic vs stochastic, linear vs nonlinear, lumped parameter vs distributed parameter, dynamic vs steady state with examples) Model building (writing down equations only)

### 2. Process Models in Chemical Engineering

Series of Isothermal, Constant- Holdup CSTRs, CSTRs with Variable Holdups, Two Heated Tanks, Gas Phase, Pressurized CSTR, Nonisothermal CSTR, Batch Reactor, Reactor with Mass Transfer, Binary Distillation Column, Problems

### 3. Numerical Methods

- Linear Algebraic Equations; Cramm's Rule, Gauss Elimination Methods, LU Decomposition, Gauss Seidal Iterative Method
- Nonlinear Algebraic Equations: Bisection Method, Newton Raphson Method, Secant Method.
- Numerical Integration: Eulers Method, Runge Kutta Method(Ist, IVth)

### 4. Simulation of single units (modules) Degrees of freedom (with and without system constraints. Coupling and decoupling of equations. Precedence ordering for Design /simulation (partitioning and tearing). Selection of design variables algorithm and persistent recycles.

### 5. Simulation of complete flow sheet. Degrees of freedom for flow sheet with connecting equations. Approaches to simulation

- Sequential modular. Precedence ordering of modules (partitioning and tearing of flow sheets)
- Simultaneous Modular with linearized modules.

### 6. Simulation Examples

Gravity Flow Tank, Three CSTR in Series, Nonisothermal CSTR, Binary Distillation Column, Batch Reactor

**Reference Books :**

1. Process Modelling, Simulation and Control for Chemical Engineers (*William Luyben*) McGraw Hill, Second Edition.
2. Chemical Process Dynamics (*John Ingham, Irvin Dunn*) VCH Publication, Cambridge.
3. Process Simulation & Control using Aspen (*Amiya K Jana*) Prentice Hall of India
4. Numerical Methods and Modelling for Chemical Engineers (*Davis M.E.*) Wiley, New York 1984
5. Basic Principles and Calculations in Chemical Engineering (*David M. Himmelblau*) Sixth Edition, Prentice Hall India.
6. Applied Mathematics in Chemical Engineering (*H.S.,Mickley.,T.S. Sherwood and C.S.Reed*) second edition, Tata MacGraw Hill New Delhi 1975
7. Process Dynamics (*Wayne Bequette*) Prentice Hall Internationals Inc., 2000
8. Systematic Methods of Chemical Process Design (*Lorenz T.Beigler, E. Ignacio Grossman and Arthur W. Westerberg*) Prentice Hall International Inc 1997
9. Numerical Methods for Engineers (*Santosh Kumar Gupta*) Tata McGraw hill, 1995

