PROCESS MODELING AND SIMULATION
(Elective-I)

Course Code: 13CH2108

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PREREQUISITES: The student should have knowledge of how to formulate differential equations in mass, momentum and heat transfer.

Course Educational Objectives:

This course teach the student

1. How to develop mathematical model for lumped and distributed parameter system
2. The concept of multiple steady stats and their stability.
3. The basic principle of dynamic optimization.

Course outcomes:

After completion of this course the student would be able to

1. Setup the model for lumped and distributed systems and solve them.
2. Understand the importance of multiple steady stats.
3. Apply the concepts of dynamic optimization to chemical engineering processes.

UNIT-I

Mathematical models for chemical engineering systems: fundamentals, introduction to fundamental laws. Examples of mathematical models of chemical engineering systems, constant hold up CSTRs, Gas pressurized CSTR, non-isothermal CSTR.

Classification of mathematical models, static and dynamic models, the complete mathematical model, Boundary conditions.

UNIT-II

Examples of single component vaporizer, Batch reactor, reactor with mass transfer, ideal binary distillation column, batch distillation with hold up.

Distributed parameter systems classification of partial differential equation.

Development of the mathematical models for

a) Tubular non-isothermal reactor.
b) Double pipe heat exchange.

UNIT-III

Solution strategies for distillated parameter systems

a) Finite difference methods: Explicit method, Crank Nicholson methods applied for a parabolic Equation in one dimension and tow dimension.

b) Finite difference method applied to Elliptic equation.

c) Orthogonal collocation method applied to a two dimensional non-isothermal packed bed reactor operation at steady state with radial dispersion.

UNIT-IV

Multiple steady states: Definition of multiple states Examples illustration multiple steady states in CSTR, bioreactor, Lorenz equations.

Stability of the steady states. Definition of steady state. Evaluation the steady state for a CSTR, bioreactor and Lorenz equation.

UNIT-V

Introduction to dynamic optimization: theory of the Pontryagins maximum principal, application of dynamic optimization to a Batch reactor problem with a reaction

A→ B→ C to maximize the concentration of B at the end of a fixed batch time.

TEXTBOOK:

1. Luyben W, "*Process Modeling, Simulation and Control for Chemical Engineers*", McGraw Hill, New York, 1990.

REFERENCE:

1. Babu B.V, *"Process Plant Simulation"*, Oxford University Press, 2001

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