PROCESS MODELING AND SIMULATION
(Elective-II)

Course Code: 15CH2110

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

Course Outcomes: On successful completion of the course, the student should be able to

CO1: Classify and develop mathematical models for chemical engineering systems.
CO2: Develop the model for lumped and distributed systems.
CO3: Solve the partial differential equations using explicit, Crank-Nicholson and orthogonal collocation methods.
CO4: Discuss the importance of multiple steady states and stability.
CO5: Apply the concepts of dynamic optimization to chemical engineering processes.

UNIT-I (10-Lectures)

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 (10-Lectures)

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 (10-Lectures)

Solution strategies for distributed parameter systems

a) Finite difference methods: Explicit method, Crank Nicholson methods applied for a parabolic equation in one dimension and two 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 (10-Lectures)

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. Evolution of the steady state for a CSTR, bioreactor and Lorenz equation.

UNIT-V (10-Lectures)

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