## CEPE3001 PROCESS SIMULATION AND MODELLING (3-0-0)

**Overall course Objective:**

The overall objective of process simulation and modeling is to gain a deep understanding of a process, enabling data-driven decision-making to optimize performance, identify inefficiencies, and test potential improvements in a safe, virtual environment before real-world implementation.

Course Outcomes

**Module - I: (10hrs)**

Introduction to process modelling and simulation, Classification: lumped vs. distributed, steady vs. unsteady, deterministic vs. stochastic. Steps in model development (assumptions, formulation, validation). Parameter estimation techniques in theoretical as well as numerical models.

Mathematical Tools for Modelling: Ordinary Differential Equations (ODEs), Partial Differential Equations (PDEs), Initial and boundary value problems, Numerical methods: Euler, Runge–Kutta, finite difference schemes, Newton–Raphson method and linear algebra for systems of equations.

**Module - II: (10hrs)**

Material & Energy balance models (Batch, CSTR, PFR models, Energy balances: isothermal and non-isothermal reactors, Thermodynamic property models, Recycle and purge streams), Transport process model.

Development of detailed mathematical models of evaporators, use of Newton Raphson method for solving evaporator problems. Separation of multi components mixtures by use of a single equilibrium stage, flash calculation under isothermal and adiabatic conditions.

Tridiagonal formulation of component material balances and equilibrium relationships for distillation, absorption and extraction of multi components. Thiele and Geddes method plus $\theta$ - method and Kb method, models of absorbers, strippers and extractors.

**Module - III: (12hrs)**

Models of Reactors: Classification of fixed bed reactor models, one dimensional and two-dimensional fixed bed reactor models, fluidized bed reactor models, bioreactor models.

Numerical Methods: Classification of partial differential equations (PDE's), solution of PDEs by Finite difference techniques, method of weighted residuals.

Process Simulation Techniques: Steady-state vs. dynamic simulation, Sequential modular and equation-oriented approaches, Numerical integration in dynamic models, Convergence and error analysis. Orthogonal collocation to solve PDEs with their application to chemical engineering systems models.

**Module - IV: (8hrs)**

Process simulation software: ASPEN Plus, HYSYS, DWSIM.

Simulation of: Distillation Column, Absorber/stripper system, Heat exchanger networks, Reactor systems, Optimization & sensitivity analysis in simulation.

**Course Outcomes**

CO1: Explain the fundamentals of process modelling, classification, and steps in model development

CO2: Develop mathematical models for chemical engineering systems (material, energy balances, transport processes)

CO3: Apply numerical techniques to solve ODEs and PDEs in process models

CO4: Simulate chemical processes using software and analyze process performance through optimization, sensitivity analysis

**Text books:**


1. Wayne Bequette – Process Dynamics: Modelling, Analysis, and Simulation.
2. Luyben W. L.,"Process Modeling Simulation and Control for Chemical Engineers", 2nd Ed., McGraw Hill, 1990.
3. William L. Luyben – Process Modelling, Simulation and Control for Chemical Engineers.


**Reference books:**


1. Aris R.,"Mathematical Modeling,Vol. 1: A Chemical Engineering Perspective (Process System Engineering)", Academic Press, 1999.
2. K. M. Hangos & I. T. Cameron – Process Modelling and Model Analysis, Academic Press, 23rd May, 2001, San Diego
3. Najim K.,"Process Modeling and Control in Chemical Engineering", CRC, 1990.