UCH802 PROCESS MODELING AND SIMULATION

L	T	P	Cr
3	0	2	4.0

Course Objectives:
To study the modeling & simulation techniques of chemical processes and to gain skills in using process simulators.

Introduction: Use and scope of mathematical modeling, Principles of model formulation, Role and importance of steady-state and dynamic simulation, Classification of models, Model building, Modeling difficulties, Degree-of-freedom analysis, Selection of design variables, Review of numerical techniques, Model simulation.

Fundamental Laws: Equations of continuity, energy, momentum, and state, Transport properties, Equilibrium and chemical kinetics, Review of thermodynamic correlations for the estimation of physical properties like phase equilibria, bubble and dew points.

Modeling of Specific Systems: Constant and variable holdup CSTRs under isothermal and non-isothermal conditions, Stability analysis, Gas phase pressurized CSTR, Two phase CSTR, Non-isothermal PFR, Batch and semi-batch reactors, Heat conduction in a bar, Laminar flow of Newtonian liquid in a pipe, Gravity flow tank, Single component vaporizer, Multi-component flash drum, Absorption column, Ideal binary distillation column and non-ideal multi-component distillation column, Batch distillation with holdup etc.

Simulation: Simulation of the models, Sequential modular approach, Equation oriented approach, Partitioning and tearing, Introduction and use of process simulation software (Aspen Plus/ Aspen Hysys) for flow sheet simulation.

Laboratory:
Writing and solving models for simple chemical processes, use of process simulator for solving models for mixer, pump, compressor, heat exchanger, reactor, absorption/distillation column and steady state flow sheet simulation.

Course Learning Outcomes (CLO):

Upon completion of this course, the students will be able to:

1. analyze physical and chemical phenomena involved in various process.
2. develop mathematical models for various chemical processes.
3. use various simulation approaches.
4. Simulate a process using process simulators (ASPEN Plus/ ASPEN Hysys).

Text Book:

1. *Luyben W.L., Process Modeling, Simulation, and Control for Chemical Engineering, McGraw-Hill (1998).*
2. *Babu, B.V., Process Plant Simulation, Oxford University Press (2004).*

Reference Books:

1. *Denn, M. M., Process Modeling, Longman Sc & Tech. (1987).*

2. *Himmelblau, D.M and Bischoff, K.B., Process Analysis and Simulation: Deterministic Systems, John Wiley (1968).*
3. *Holland, C. D., Fundamentals and Modeling of Separation Processes: Absorption, Distillation, Evaporation and Extraction, Englewood Cliffs, Prentice-Hall (1974).*

Evaluation Scheme:

S. No.	Evaluation Elements	Weightage (%)
1	MST	25
2	EST	40
3	Sessional (may includes tutorials/ assignments/ quiz's etc)	35