Gyanmanjari Innovative University

Course Syllabus
Gyanmanjari Institute of Technology
Semester-7

Subject: Process Simulation & Optimization- BETCH17328

Type of course: Major (Core)

Prerequisite: Basic knowledge of Chemical Reaction Engineering, thermodynamics, and transport phenomena, along with familiarity with mathematical modeling.

Rationale: This course introduces simulation and optimization techniques for analyzing and improving chemical processes. It covers modeling of reactors and process systems, including non-ideal and non-isothermal behavior, to enhance efficiency, performance, and economic viability in industrial applications.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks					Total Marks
CI	T	P	C	Theory Marks		Practical Marks		CA	
				ESE	MSE	V	P	ALA	
4	0	2	5	60	30	10	20	30	150

Legends: CI-Classroom Instructions; T – Tutorial; P - Practical; C – Credit; ESE – End Semester Examination; MSE- Mid Semester Examination; CA - Continuous Assessment; ALA-Active Learning Activities.

Course Content:

Sr. No	Course content	Hrs	% Weightage
1	**Introduction and Process Design Concepts:** Overview of chemical process engineering, Stages of process design: Process synthesis, Process analysis, Optimization. Concept of flow sheeting and simulation, Role and applications of process simulation in industry, Design mode vs analysis mode of simulation, Introduction to computer-aided process design.	10	10

2	**Modelling Fundamentals and Mathematical Models:** Deterministic and stochastic processes, Physical and mathematical modelling, Model formulation using fundamental laws (mass, energy, momentum), Principles of similarity (geometric, kinematic, dynamic), Classification of models: Lumped vs distributed, Static vs dynamic, Deterministic vs probabilistic. Boundary conditions and black-box modelling, Introduction to Artificial Neural Networks (ANN).	10	20
3	**Modelling of Chemical Engineering Systems:** Mass Transfer Models: Solvent extraction, gas absorption, distillation. Heat Transfer Models: Steady and unsteady heat conduction, Heat exchangers and extended surfaces. Fluid Flow Models: Continuity equation, flow through packed beds and pipes. Reaction Engineering Models: Reactor modelling (PFR, packed bed), Reaction with heat and mass transfer.	15	30
4	**Data Analysis and Optimization Techniques:** Experimental data analysis and error propagation, Data regression and curve fitting methods, Objective functions and constraints, Traditional optimization techniques: Lagrange multipliers, Gradient methods. Non-traditional optimization techniques: Genetic algorithms, Simulated annealing, Differential evolution.	10	20
5	**Process Simulation Methods and Software** Modular approach to simulation, Equation-solving approach, Network decomposition and tearing algorithms, Convergence techniques (Newton, Wegstein, etc.), Physical and thermodynamic property estimation, Steady-state and dynamic simulation. Case studies: reactors, heat exchangers, pyrolysis. Introduction to simulation software: ASPEN PLUS	15	20

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Continuous Assessment:

Sr. No	Active Learning Activities	Marks
1	**Basic Process Simulation:** Simulate a simple process such as mixing of two streams, heater/cooler, or flash drum using simulation software. Perform basic material and energy balance and observe output conditions (temperature, composition). Submit simulation file and short report on the GMIU Web Portal.	10
2	**Simple Optimization Study:** Using the above simulation, vary one parameter (e.g., temperature, pressure, or flow rate) to find better operating conditions. Submit report on the GMIU Web Portal.	10
3	**Mini Simulation Case Study:** Simulate a basic unit operation such as a heat exchanger or simple distillation column in simulation software. Analyze performance (temperature change, energy duty, composition) and suggest one or two improvements. Submit a short report with screenshots on the GMIU Web Portal.	10
	Total	30

Suggested Specification table with Marks (Theory): 60

Distribution of Theory Marks (Revised Bloom's Taxonomy)						
Level	Remembrance (R)	Understanding (U)	Application (A)	Analyze (N)	Evaluate (E)	Create (C)
Weightage	20%	20%	20%	20%	20%	0%

Note: This specification table shall be treated as a general guideline for students and teachers. The actual distribution of marks in the question paper may vary slightly from above table.

Course Outcome:

After learning the course, the students should be able to:	
CO1	Understand process design concepts and simulation fundamentals
CO2	Develop mathematical models for chemical engineering systems
CO3	Analyze process performance using simulation techniques
CO4	Apply optimization methods to improve process efficiency
CO5	Use simulation software for solving industrial process problems

List of Suggested Practical

Sr. No	Suggested Practical	Unit No	Hrs.
1	To simulate mixing of two streams and perform material balance using simulation software.	1	4
2	To simulate a heater/cooler and analyze energy balance and temperature changes.	1	4
3	To simulate a flash drum and study vapor-liquid equilibrium.	3	4
4	To simulate a simple distillation column (binary system) and analyze separation efficiency.	3	4
5	To study the effect of operating parameters (temperature/pressure) on process performance using simulation software.	4	4
6	To perform basic optimization by varying one parameter to improve purity or reduce energy consumption.	4	6
7	To simulate a heat exchanger and evaluate heat duty and effectiveness.	5	4

Instructional Method:

The course delivery method will depend upon the requirement of content and the needs of students. The teacher, in addition to conventional teaching methods by black board, may also use any tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.

From the content 10% topics are suggested for flipped mode instruction. Students will use supplementary resources such as online videos, NPTEL/SWAYAM videos, e-courses. The internal evaluation will be done on the basis of Active Learning Assignment.

Practical/Viva examination will be conducted at the end of semester for evaluation of performance of students in the laboratory.

Reference Books:

[1] B.V. Babu, Process Plant Simulation, Oxford University Press, 2004.
[2] W.L. Luyben, Process Modeling, Simulation and Control for Chemical Engineers, McGraw-Hill, 2nd Edition, 1990.
[3] B. Wayne Bequette, Process Control: Modeling, Design, and Simulation, Prentice Hall, 2003.
[4] R. Turton, R.C. Bailie, W.B. Whiting & J.A. Shaeiwitz, Analysis, Synthesis, and Design of Chemical Processes, Prentice Hall, 4th Edition, 2012.
[5] S. Seider, J.D. Seader, D.R. Lewin & S. Widagdo, Product and Process Design Principles, Wiley, 3rd Edition, 2010.
[6] E. Edgar, D.M. Himmelblau & L.S. Lasdon, Optimization of Chemical Processes, McGraw-Hill, 2nd Edition, 2001.