GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL ENGINEERING (COMPUTER AIDED PROCESS DESIGN) (16)
CHEMICAL SYSTEM MODELING & SIMULATION
SUBJECT CODE: 2711608
SEMESTER: I

Type of course: Maths relevant Branch (M.E.CAPD)

Prerequisite: --

Rationale: --

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks						Total Marks
				Theory Marks		Practical Marks				
L	T	P	C	ESE (E)	PA (M)	PA (V)		PA (I)		
						ESE	OEP	PA	RP	
3	2	0	4	70	30	30	0	10	10	150

Content:

Sr. No.	Topics	Teaching Hrs.	Module Weightage
1	**Modeling Aspects :** Deterministic Versus Stochastic Process, Deterministic Process, Stochastic Process, Physical Modeling, Mathematical Modeling.	06	10
2	**Classification of Mathematical Modeling:** Independent and Dependent Variables, and Parameters, Classification based on Variation of Independent Variables, Distributed parameter Models, Lumped Parameter Models, Classification based on the State of the Process, Static Model, Dynamic Model, The complete Mathematical Model, Classification Based on the Type of the Process, Rigid or Deterministic Models, Stochastic or Probabilistic Models, Comparison between Rigid and Stochastic Model.	06	15
3	**Models in Mass-Transfer Operations:** Steady–state Single–stage Solvent Extraction, Steady-state Two–stage Solvent Extraction, Steady-state N–stage Counter-current Solvent Extraction.	06	15
4	**Models in Heat –transfer Operations:** Counter current Cooling of Tanks, Temperature Distribution in a Transverse Cooling fin of Triangular Cross-Section, Unsteady-state heat Transfer in a Tubular Gas Pre heater, Heat loss through pipe flanges.	06	10
5	**Models in Fluid-flow Operations:** **Laminar** flow in a Narrow slit, The Continuity Equation, Concentration Profile and Temperature of fixed bed catalytic Reactor.	06	10
	Simulation:		
6	**Modular Approaches & Equation:** Modular Approaches to process simulation, The Equation solving approach.	06	10
7	**Decomposition of networks :**	06	10

	Tearing algorithms, Algorithms based on the signal flow graph, Algorithms based on reduced diagraph.		
8	**Convergence promotion and physical and thermodynamic properties:** Convergence promotion, Physical and thermodynamic properties.	06	10
9	**Professional simulation packages:**	06	10

Reference Books:
1. Systematic Methods of Chemical Process Design, Lorens T. Biegler , E.Ignacio grossmann, Arthur W Westerberg, Prentice Hall International,Inc
2. Process Plant Simulation --- B.V.Babu
3. Applied Mathematics in Chemical engg---- Mickley, Sherwood & Reed
4. Mathematical methods in Chemical engg---- Jenson & Jeffereys
5. Chemical Sy Modeling and Simulation by Lyuben

Course Outcome:

After learning the course the students should be able to:

1. Develop the Physical Modeling & Mathematical Modeling.
2. Comparison between Rigid and Stochastic Model.
3. Develop the models for Mass Transfer Operation.
4. Develop the models for Heat Transfer Operation.
5. Develop the models for Fluid Flow Operation.
6. Design the Algorithms based on the signal flow graph.
7. Design the Algorithms based on reduced diagraph.
8. Learnt the professional Simulation Packages.
9. Create Modular Approaches to process simulation.

List of Open Source Software/learning website:

- www.sciencedirect.com/science/article/pii/S0167642304001935
- www.autodesk.in/products/autodesk-simulation-family/overview
- www.bits-pilani.ac.in/uploads/Chemical_Courses.pdf
- www.scribd.com/doc/.../106487559-Process-Plant-Simulation-Babu
- www.scribd.com/doc/44822675/07-Chemical-Process-Simulation