

GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL (COMPUTER AIDED PROCESS DESIGN) (16)

CHEMICAL SYSTEM MODELING AND SIMULATION

SUBJECT CODE: 3711608

SEMESTER: I

Type of course: Core 1

Prerequisite: Mass Transfer fundamentals

Rationale: The aim of this subject is to impart comprehensive understanding to the students regarding various novel and advanced separation techniques and its advancement which have profound significance in Industrial and Research arenas.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks				Total Marks
L	T	P		Theory Marks		Practical Marks		
			ESE(E)	PA (M)	PA (V)	PA (I)		
3	0	4	5	70	30	30	20	150

Content

Sl. No.	Topic	Teaching Hours	Module Weightage (%)
1	Modeling Aspects : Deterministic Versus Stochastic Process, Deterministic Process, Stochastic Process, Physical Modeling, Mathematical Modeling.	6	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.	6	10
3	Models in Mass-Transfer Operations: Steady-state Single-stage Solvent Extraction, Steady-state Two-stage Solvent Ext	6	10
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.	6	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.	6	10

	Simulation		
6	Modular Approaches & Equation: Modular Approaches to process simulation, The Equation solving approach.	6	10
7	Decomposition of networks : Tearing algorithms, Algorithms based on the signal flow graph, Algorithms based on reduced diagraph.	6	10
8	Convergence promotion and physical and thermodynamic properties: Convergence promotion, Physical and thermodynamic properties.	6	10
9	Professional simulation packages:	6	20
	Total	54	100

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 Experiments:

Suitable experiments based on programming and usage of programs like C, MATLAB, SCILAB, GAMS etc. Usage of simulation packages/softwarewares like ASPEN, Design-II etc and experiments on application in chemical engineering

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