



GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Master of Engineering

Level: PG

Branch: Computer Aided Process Design

Course / Subject Code: ME01072011

Course / Subject Name : Chemical System Modelling and Simulation

w. e. f. Academic Year:	2024-25
Semester:	1 st Semester
Category of the Course:	PCC

Prerequisite:	Basic knowledge of modelling and simulation
Rationale:	To provide students an insight of modelling aspects in chemical engineering. To provide students knowledge about simulation in chemical systems To understand and apply the simulation softwares currently used in chemical engineering.

Course Outcome:

After completion of the course, student will able to:

No	Course Outcomes
01	Understand the modelling aspects and different types of models
02	Develop the models for mass transfer operation, heat transfer operation, fluid flow operations and reactors
03	Understand the concept of simulation
04	Develop the algorithms based on the signal flow graph and digraph
05	Construct and interpret process flowsheets using professional simulation packages.

Teaching and Examination Scheme:

Teaching Scheme(in Hours)			Total Credits L+T+(PR/2)	Assessment Pattern and Marks				Total Marks
L	T	PR		C	Theory		Tutorial / Practical	
			ESE (E)		PA / CA (M)	PA/CA (I)	ESE (V)	
3	0	2	4	70	30	20	30	150



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Course Content:

UnitNo.	Content	No. of Hours	% of Weightage
1.	Modelling Aspects : Physical Modelling, Mathematical Modelling, Deterministic process, Stochastic Process, Model Formulation Principles, Fundamental Laws used in Modelling, chemical system modelling.	4	10
2.	Classification of Mathematical Modelling: Independent and Dependent Variables and Parameters, Classification based on - Variation of Independent Variables, State of the Process, Type of the Process, Boundary conditions, Black box principles, Artificial neural networks.	4	10
3.	Models in Mass-Transfer Operations: Steady-state Single-stage and two-stage Solvent Extraction, Steady-state Two-stage Cross-current solvent extraction, Unsteady-state Single-stage Solvent Extraction, Steady-state N-stage Counter-current Solvent Extraction, Unsteady-state Mass Balance in a Stirred Tank, Multistage Gas Absorption (Kremser-Brown Equation), Multistage distillation	5	10
4.	Models in Heat –transfer Operations: Steady-state Heat Conduction Through Hollow Cylindrical Pipe, Counter current Cooling of Tanks, Unsteady-state Steam Heating of a Liquid, Heat loss through pipe flanges, Unsteady-state heat Transfer in a Tubular Gas Pre heater, Unsteady-state Heat Transfer by Conduction.	5	10
5.	Models in Fluid-flow Operations: Laminar flow in a Narrow slit, The Continuity Equation, Flow Through a Packed Bed Column, Laminar Flow in a Narrow Slit.	4	10
6.	Models in Reaction Engineering: Modelling of Tubular reactor, Batch reactor, CSTR, Packed bed reactor.	4	10
7.	Introduction to simulation: Analysis vs design mode, Modular approaches and equation solving approach, Boolean Adjacency matrices, digraphs & signal flow graphs, Path tracing methods, sparse systems,	5	10
8.	Decomposition of networks : Tearing algorithms, Algorithms based on the signal flow graph, Algorithms based on reduced digraph, comparison of algorithms	5	10



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9.	Convergence promotion and physical and thermodynamic properties: Convergence promotion along with the methods, Physical and thermodynamic properties-source, databanks, modularity & routing.	4	10
10.	Professional simulation packages: Specific-purpose simulation and dynamic simulation, professional simulation packages used in chemical engineering.	5	10
Total		45	100

Suggested Specification Table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
10	15	15	15	10	5

Where R: Remember; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create (as per Revised Bloom's Taxonomy)

References/Suggested Learning Resources:

(a) 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, Oxford University Press
3. Process Modelling and Simulation for Chemical Engineers by Simant Ranjan Upreti, Wiley Publication, 2017
4. Mathematical methods in Chemical Engg---- Jenson & Jeffereys
5. Chemical System Modelling and Simulation by Lyuben, McGraw Hill Publication

(b) Open source software and website:

1. NPTEL open course on ASPEN simulation (<https://nptel.ac.in/courses/103103209>)
2. NPTEL open course on Process modelling and simulation (<https://archive.nptel.ac.in/courses/103/107/103107096/>)
3. Open source software DW-SIM,
4. Open source compiler SCILAB, C, C++



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Suggested Course Practical List:

Experiments based on the following:

- Computations based on programming languages like C, C++, MATLAB, SCILAB etc.
- Usage of simulation packages/software like ASPEN, ChemCAD, Design-II, DW-SIM etc.
- Validation of models based on chemical systems with data generated from actual experiments.

Suggested Activities for Students:

1. Use of C, MATLAB, SCILAB etc. or any other computing language to make programs/spreadsheets based on above topics.
2. Application of above methods to solve problems related to chemical engineering.
