



SARVAJANIK
UNIVERSITY

INCLUSIVE | INTEGRATED | INNOVATIVE

SARVAJANIK UNIVERSITY
Sarvajani College of Engineering and Technology



Bachelor of Technology (B.Tech)

B.Tech. Semester VII

Subject Name: Modeling and Simulation in Chemical Engineering

Subject Code: BTCH14701

Type of course: Professional Elective Course

Prerequisite: Maths, Numerical Techniques, Mathematical methods, Basic calculations in chemical engineering, Chemical Reaction Engineering-I, Fluid Flow Operations, Heat Transfer Operations, Mass transfer Operations I & II, Chemical Engineering Thermodynamics – I & II

Rationale: This course offers basic understanding for modeling and simulation of important steps for process synthesis such as reactors, heat exchangers, separation operations, fluid moving devices.

Teaching and Examination Scheme:

TEACHING SCHEME				Theory Marks			Practical Marks		Total
L	T	P	C	TEE	CA1	CA2	TEP	CA3	150
3	0	2	4	60	25	15	30	20	

CA1: Continuous Assessment (assignments/projects/open book tests/closed book tests CA2: Sincerity in attending classes/class tests/ timely submissions of assignments/self-learning attitude/solving advanced problems TEE: Term End Examination TEP: Term End Practical Exam (Performance and viva on practical skills learned in course) CA3: Regular submission of Lab work/Quality of work submitted/Active participation in lab sessions/viva on practical skills learned in course

Content:

Sr. No	Topics	Teaching Hrs.	Module Weightage
1.	Introduction of Modeling: Introduction to chemical Engg system models, Modeling Aspects, Classification of Mathematical Modeling, Model development procedure: system analysis, modeling, simplification of model, solution and validation.	4	9
2.	Mathematical Models of Chemical Engineering Systems: Introduction, uses of mathematical models, scope of coverage, principles of formulation, fundamental laws: continuity equations, energy equations, equation of motion, transport equation, equation of state, equilibrium, kinetics.	6	14
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, ideal binary distillation column, batch distillation with holdup,	7	16
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.	4	9
5.	Models in Fluid-flow Operations: Laminar flow in a Narrow slit, The Continuity Equation, Concentration Profile and Temperature of fixed bed catalytic Reactor.	4	9
6.	Models for Reactors: series of isothermal, constant-hold up CSTR, CSTR with variable holds up, gas-phase, pressurized CSTR, non-isothermal CSTR, single-component vaporizer, batch reactor, reactor	5	12





	with mass transfer		
7.	Introduction to Simulation : various approaches – modular and equation solving	3	7
8.	Decomposition of network : tearing and partitioning algorithms	5	12
9.	Software used for chemical process simulation : Professional simulators and equation solvers.	3	7
10.	Specific Applications of simulation : Ammonia synthesis reactor, Thermal cracking operation, Design of shell and tube heat exchanger, pyrolysis of biomass	4	9

Suggested Specification table with Marks (Theory/Practical):

% Distribution of Marks					
R Level	U Level	A Level	N Level	E Level	C Level
15	20	20	5	00	00

Legends: R: Remembrance, U: Understanding; A: Application, N: Analyze, E: Evaluate C: Create and above Levels (**Revised Bloom's Taxonomy**)

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.

Reference Text Books:

Sr. No.	Title of book /article	Author(s)	Publisher and details like ISBN	Year of publication	Publication Edition
1.	Process Modeling, Simulation and Control for Chemical Engineers	William L. Luyben	McGraw Hill ISBN 0070391599, 9780070391598	1990	2 nd Editions
2.	Process plant simulations	B. V. Babu	Oxford University Press ISBN: 9780195668056, 0195668057	2004	-
3.	Process Dynamics: Modeling, Analysis and Simulation	B Wayne Bequette	Prentice Hall International Inc ISBN: 9780132068895, 0132068893	1998	-
4.	Systematic Methods of Chemical Process Design	Lorenz T. Biegler, E. Ignacio grossmann, Arthur W. Westerberg	Prentice Hall International ISBN-0134924223, 9780134924229	2007	-
5.	Mathematical Methods in Chemical Engineering	Jenson, V.G. and Jeffreys, G.V.	Academic Press/ Elsevier Science ISBN: 0-12-384456-8	1963/1977	2 nd edition
6.	Process Modeling	Denn M. M.	Longman	1986	-
7.	Fundamentals and Modeling of Separation processes	Holland C. D.	Prentice Hall., ISBN: 9780133443905, 0133443906	1975	-
8.	Mathematical Modeling Vol.1: A Chemical Engineering Perspective (Process System Engineering)	Rutherford Aris	Academic Press Elsevier ISBN: 0080511244, 9780080511245	1999	-
9.	Process Modeling and Simulation for Chemical Engineers: Theory and	Simant R. Upreti	Wiley ISBN: 978-1-118-91466-3	2017	-





Practice				
----------	--	--	--	--

Course Outcome:

Sr. No.	CO Statement After learning this subject, students will be able to	Marks % weightage
CO-1	Understand the chemical engineering system and should be able to identify the system parameters.	10
CO-2	Enlist the mathematical correlations between the parameters of the system.	15
CO-3	Develop a mathematical model for the chemical processes and operations.	25
CO-4	Decide the sequence of solving the equations using fundamentals of tearing and partitioning.	25
CO-5	Simulate the chemical systems using software and interpret the results obtained.	25

Mapping with Pos:

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	P O1 0	PO 11	P O1 2	PS O1	PS O2	PS O3
CO-1	3	3	3	2	3	3	3	3	3	3	2	3	3	3	3
CO-2	3	3	3	3	3	3	3	3	3	2	3	3	2	3	3
CO-3	2	3	3	3	2	3	2	2	3	3	3	3	3	3	3
CO-4	3	3	2	3	3	3	3	2	3	2	3	3	3	3	3
CO-5	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
Rationale*	14	15	14	14	14	15	14	13	15	13	14	15	14	15	15

Rationale*: Explaining why it is matching this particular program outcome

LIST OF PRACTICALS: (Minimum 10 to be performed.)

Sr No	Experiment
	Develop the model for following processes/operations and compare the results obtained by model equation with the results obtained by simulation in software and conclude.
1	Reactors: CSTR, PFR
2	Separators: Distillation, rigorous distillation, Absorption, Extraction, drying, flash operation
3	Heat exchanger: Shell and Tube, Evaporator, Condenser

Major Equipment: Computers with specifications compatible to run the softwares.

List of Open Source/learning website:

- <https://nptel.ac.in/courses/103/107/103107096/> : web course on Process Modeling and Simulation by Dr. V. K. Agrawal, IIT Roorkee.
- www.scilab.in (free literature for solution of books for chemical engineering)

List of Open Source Software: Computer with software i.e. MS Excel, Scilab, Python, DWSIM, ChemCAD/ASPEN one etc.

