Subject Code: 01CH0701
Subject Name: Process Modelling & Simulation
B. Tech. Year – IV (Semester VII)

Objective: The course is intended to identify the suitable modelling and simulation approach for various chemical engineering operations.

Credits Earned: 4 Credits

Course Outcomes: After completion of this course, student will be able to:

1. Identify the suitable process modelling approach for various processes.
2. Construct the mathematical modelling for different processes.
3. Plan the appropriate modelling and simulation methodology for respective system.
4. Test and justify the developed model for a particular process.
5. Design and rearrange the parameters based on the modelling approach.

Pre-requisite of course: Fluid Flow Operations, Chemical Reaction kinetics, Engineering Mathematics

Teaching and Examination Scheme

Teaching Scheme (Hours)			Credits	Theory Marks			Tutorial/ Practical Marks		Total Marks
Theory	Tutorial	Practical		ESE (E)	IA (I)	CSE (C)	Viva (V)	Term work (TW)	
3	0	2	4	50	30	20	25	25	150

Contents:

Unit	Topics	Contact Hours
1	**Modelling Fundamentals** Uses of Mathematical models; Deterministic versus stochastic processes; Physical modelling, Mathematical modelling; Principles of formulation; Fundamental Laws – Continuity equation, Energy equation, Equation of Motion, Transport equation, Equations of state, Equilibrium, Chemical Kinetics, Strategy of process engineering	5
2	**Classification of Mathematical Modelling** Variables and parameters; Classification based on variation of independent variables; Classification based on the state of process; Classification based on the type of the process; Boundary Conditions; The black box principle; Artificial	5

	Neural Network	
3	**Models in Mass-Transfer Operations** Steady-state single-stage solvent extraction; Steady-state two-stage solvent extraction; Steady-state two-stage cross-current solvent extraction; Unsteady-state single-stage solvent extraction; Unsteady state mass balance in a stirred tank; Unsteady state mass balance in a mixing tank; Batch Distillation with holdup; Reactor with mass transfer	10
4	**Models in Heat-Transfer Operations** Two heated tanks; Steady-state heat conduction through a hollow cylindrical pipe; Unsteady-state steam heating of a liquid; Unsteady-state heat loss through a maturing tank; Counter-current cooling of tanks; Heat transfer through extended surfaces; Unsteady-state heat transfer in a tubular gas preheater; Heat loss through pipe flanges; Heat transfer in thermometer system	10
5	**Models in Fluid-flow operations** The continuity equation; Flow through a packed bed column; Laminar flow in a narrow slit; Flow of a film on the outside of a circular tube; Parallel-disc viscometer	6
6	**Process Modelling Software – Professional simulation packages** Introduction; Ansys; Aspen; Comsol; Case studies.	3
	Total Hours	**39**

List of Experiments:

1. To perform various data operations in SCILAB
2. To perform matrix calculations using SCILAB
3. To plot various graphs in SCILAB.
4. To obtain for solution for ordinary differential equation of first order in reaction kinetics using SCILAB.
5. To perform Matrix calculations in Matlab.
6. To plot curve using plot function in Matlab.
7. To fit curves in Matlab.
8. To calculate Hessian matrix using Matlab.

Reference Text Books:

1. William L. Luyben, Process Modeling, Simulation and Control for Chemical Engineers, McGraw Hill International Editions
2. B. V. Babu, Process Plant Simulations, Oxford University Press.

Suggested Theory distribution:

The suggested theory distribution as per Bloom's taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery and evaluation					
Remember	Understand	Apply	Analyze	Evaluate	Create
10	20	25	25	10	10

Instructional Method:

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

b. The internal evaluation will be done on the basis of continuous evaluation of students in the laboratory and class-room.

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

d. Students will use supplementary resources such as online videos, NPTEL videos, e-courses, Virtual Laboratory

Design Based Problems (DP)/ Open Ended project (OEP):

In the beginning of the session, subject faculty will allot an OEP / DP to the students. Students will be free to choose a topic of their choice which will be relevant to the syllabus and they will either prepare a working model/ report / presentation / poster on their topic.

Online Web Resources:

1. http://www.prosim.net/en/index.php
2. https://www.chemstations.com/CHEMCAD/
3. https://www.aspentech.com/en/products/engineering/aspen-plus
4. https://chengineer.in/