

GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL ENGINEERING (30) PROCESS MODELLING & SIMULATION SUBJECT CODE: 2723011 SEMESTER: II

Type of course: Chemical Engineering (Major Elective-II)

Prerequisite: Fundamental of Process Engineering & Engineering Mathematics.

Rationale: The Process Modeling and Simulation of Chemical engineering processes has attracted the attention of scientists and engineers for many decades and is still a subject of major importance for the knowledge of transport processes and its kinetics.

Basically it deals with three aspects, namely: modeling of chemical engineering processes, parameter estimations and application of numerical methods for solution of models.

This subject includes the concepts of modeling, optimization, decomposition of networks, modular and equation solving approaches, data regression, convergence promotion, specific-purpose simulation and dynamic simulation etc.

Teaching and Examination Scheme:

Teaching Scheme			Credits C	Examination Marks						Total Marks
L	T	P		Theory Marks		Practical Marks				
			ESE (E)	PA (M)	ESE (V)		PA (I)			
					ESE	OEP	PA	RP		
3	2#	2	5	70	30	20	10	10	10	150

Content:

Sr. No.	Content	Total Hrs	%Weightage
1	Modelling Aspects Definition of process model, Physical and Mathematical modelling, Deterministic and Stochastic process, Classification of models, Model building, Black-box model, White box model, Gray model, Classification of Mathematical methods,	7	13
2	Mathematical methods 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	10	18
3	Examples of mathematical models of chemical engineering systems Introduction, Series of Isothermal, Constant-Hold up CSTRs, CSTRs with variable Holds up, Two heated tanks, Gas-phase, Pressurized CSTR, Nonisothermal CSTR, Single-Component vaporizer, Multicomponent Flash drum, Batch Reactor, Reactor with Mass transfer, Ideal Binary distillation column, Multicomponent non ideal Distillation column, Batch	16	30

	distillation with holdup		
5	Simulation: Degree of freedom analysis, Types of simulation problems: Design, Rating, Flow sheeting etc. Usefulness and Limitation of Process Simulation.	7	13
6	Partitioning and Tearing Steady State Lumped System-Partitioning Equation, Tearing Equation, Simultaneous Equation, Modular Approaches & Equation Solving Approaches, Decomposition of Networks.	8	15
7	Introduction to various professional simulators and equation solver software.	6	11

Reference Books:

1. Process Dynamics: Modeling, Analysis and Simulation, B Wayne Bequette, Prentice Hall International Inc.
2. Process Plant Simulations, B V Babu, Gulf Publications
3. Process Modelling, Simulation and Control for Chemical Engineers by William L. Luyben, McGraw Hill International Editions.
4. Analysis, Synthesis and Design of Chemical Processes, R Turton, R C Bailie, W B Whiting and J A Shaeiwitz, Prentice Hall International In.
5. Product and Process Desing Principles-Synthesis, Analysis, and Evaluation, 2nd ed., W D Seider, J D Seader and D R Lewin, John Wiley and Sons Inc.

Course Outcome:

After learning the course the students should be able to:

- Development of process models based on conservation principles and process data.
- Simulate the chemical processes and different parts of the processes.
- Carry out simulation of unit operations.
- Hands on exposure of professional simulation software will make them ready for industry.
- Have an understanding of computational techniques to solve the process models.
- Use simulation tools such as MATLAB, SCILAB etc.

LIST OF PRACTICALS AND OPEN ENDED PROJECTS :

Minimum 5 practical's to be performed and remaining Open-ended Projects / Study Reports / Latest outcomes in technology study :-

1. In the beginning of the academic term, faculties will have to allot their students at least one Open-ended Projects / Study Reports / Latest outcomes in technology. Literature survey including patents and research.
 - Design based small project **or**
 - Study report based on latest scientific development **or**
 - Technology study report/ modeling/ simulation/collection report **or**
 - Computer based simulation/ web based application/ analysis presentations of applied science field which may help them in their branches especially in their UDP/IDP projects.
2. These can be done in a group containing maximum three students in each.
3. Faculties should cultivate problem based project to enhance the basic mental and technical level of students.
4. Evaluation should be done on **approach of the student on his/her efforts** (not on completion) to study the design module of given task.

5. In the semester student should perform **minimum 5 set of experiments** and complete **one small open ended project** based on engineering applications. This project along with any performed experiment should be **EVALUATED BY EXTERNAL EXAMINER.**

List of Open Source Software/learning website:

- Students can refer to video lectures available on the websites including NPTEL lecture series.
- Students can refer to the CDs available with some reference books for the solution of problems using software/spreadsheets. Students can develop their own programs/spreadsheets for the solution of problems.

ACTIVE LEARNING ASSIGNMENTS:

The tutorials will be given to students which will cover entire content of the subject. The students will be required to solve all problems given in the tutorials. Some of the problems they have to solve using programming language or software. The list is given below:

- Aspan Hysys
- Chemcad
- Super-pro Designer
- Excel Spreadsheets
- Polymath
- Matlab/Scilab, etc.

Review Presentation (RP): The concerned faculty member shall provide the list of peer reviewed Journals and Tier-I and Tier-II Conferences relating to the subject (or relating to the area of thesis for seminar) to the students in the beginning of the semester. The same list will be uploaded on GTU website during the first two weeks of the start of the semester. Every student or a group of students shall critically study 2 papers, integrate the details and make presentation in the last two weeks of the semester. The GTU marks entry portal will allow entry of marks only after uploading of the best 3 presentations. A unique id number will be generated only after uploading the presentations. Thereafter the entry of marks will be allowed. The best 3 presentations of each college will be uploaded on GTU website