GUJARAT TECHNOLOGICAL UNIVERSITY

BRANCH NAME: CHEMICAL ENGINEERING
SUBJECT NAME: PROCESS MODELING, SIMULATION & OPTIMIZATION
SUBJECT CODE: 2180503
B.E. 8th SEMESTER

Type of course: Chemical Engineering

Prerequisite: Basic Knowledge of Unit Operations, Fundamental of Process Engineering and Engineering Mathematics.

Rationale: The Process Modeling, Simulation and Optimization of chemical engineering processes is a subject of major importance for the knowledge of transport processes; improved design process and its kinetics. Basically this subject comprises of three parts; modeling, simulation and optimization. Modeling and simulation emphasize on the concept of modeling of chemical engineering processes, parameter estimations, decomposition of networks, application of numerical methods, data regression, convergence promotion, specific-purpose simulation, dynamic simulation, etc. Optimization includes the concept; i.e., how one develops mathematical statements for the objective function (usually economic model) to be minimized or maximized and the equality and inequality constraints (the process model) and selection of optimization technique which is best suited to the problem characteristics.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks						Total Marks
				Theory Marks			Practical Marks			
L	T	P	C	ESE (E)	PA (M)		ESE (V)		PA (I)	
					PA	ALA	ESE	OEP		
4	0	3	7	70	20	10	20	10	20	150

Content:

Sr. No.	Content	Total Hrs	% Weightage
	CHEMICAL PROCESS MODELING		
1	**Modeling Aspects:** Definition of process model, physical and mathematical modeling, deterministic and stochastic process, classification of models, model building, black-box model, white box model, gray model, classification of mathematical methods.	6	8
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	7	10

	state, equilibrium, kinetics.		
3	**Examples of Mathematical Models of Chemical Engineering Systems:** Introduction, series of isothermal, constant-hold up CSTR, CSTR with variable holds up, two heated tanks, gas-phase, pressurized CSTR, non-isothermal CSTR, single-component vaporizer, batch reactor, reactor with mass transfer, ideal binary distillation column ,batch distillation with holdup.	**11**	**16**
CHEMICAL PROCESS SIMULATION			
4	**Partitioning and Tearing:** Steady state lumped system-partitioning equation, tearing equation, simultaneous equation, modular approaches & equation solving approaches, decomposition of networks.	**6**	**8**
5	**Introduction to Various Professional Simulators and Equation Solver Software:**	**3**	**4**
CHEMICAL PROCESS OPTIMIZATION			
6	**The Nature and Organization of Optimization Problems:** Scope and hierarchy of optimization, examples of applications of optimization, the essential features of optimization problems, general procedure for solving optimization problems, obstacles to optimization.	**4**	**6**
7	**Developing Models for Optimization:** Classification of models, how to build a model, selecting functions to fit empirical data, factorial experimental designs, degrees of freedom, examples of inequality and equality constrains in models, formulation of the objective function.	**6**	**8**
8	**Basic Concepts of Optimization:** Continuity of function, NLP problem statement, convexity and its applications, interpretation of the objective function in terms of its quadratic approximation, necessary and sufficient conditions for an extremum of an unconstrained function.	**6**	**8**
9	**Optimization of Unconstrained Functions:** One-Dimensional search numerical methods for optimizing a function of one variable, scanning and bracketing procedures, Newton and Quasi-Newton methods of uni-dimensional search, polynomial approximation methods, how one-dimensional search is applied in a multidimensional problem, evaluation of uni-dimensional search methods.	**6**	**8**
10	**Unconstrained Multivariable Optimization:** Methods using function values only, methods that use first derivatives, Newton's method, Quasi-Newton methods.	**4**	**6**

11	**Linear Programming (LP) and Applications:** Geometry of linear programs, basic linear programming, definitions and results, simplex algorithm.	**5**	**7**
12	**Non Linear Programming (NLP) and Applications:** Penalty and Lagrange's method, etc.	**3**	**4**
13	**Application of Optimizations:** Examples of optimization in chemical processes like: optimizing recovery of waste heat, optimal shell and tube heat exchanger design, optimal design and operation of binary distillation column, chemical reactor design and operation.	**5**	**7**

Suggested Specification table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
14	14	28	7	7	0

Legends: R: Remembrance; U: Understanding; A: Application, N: Analyze and 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 Books:

1. B Wayne Bequette, Process Dynamics: Modeling, Analysis and Simulation, Prentice Hall International Inc.
2. B V Babu, Process Plant Simulations, Gulf Publications.
3. William L. Luyben, Process Modeling, Simulation and Control for Chemical Engineers, McGraw Hill International Editions.
4. R Turton, R C Bailie, W B Whiting and J A Shaeiwitz, Analysis, Synthesis and Design of Chemical Processes, Prentice Hall International In.
5. W D Seider, J D Seader and D R Lewin, Product and Process Design Principles-Synthesis, Analysis, and Evaluation, 2nd ed., John Wiley and Sons Inc.
6. Edger, Himmelblau, Lasdon, Optimization of Chemical Processes, McGraw-Hill International Edition.
7. Gordon S. G. Beveridge and Rober S. Schechter, Optimization: Theory and Practice, McGraw-Hill Book Company.
8. K. Deb, Optimization for Engineering Design, Prentice-Hall.
9. MC Joshi and K M Moudgalya, Optimization: Theory and Practice, Narosa Publishing, ISBN: 81-7319-424-6.
10. Nocedal and S J Wright, Numerical Optimization, Springer Verlag. , ISBN:0-387-98793-2.
11. Dimitris Bertsimas, John N. Tsitsiklis, John Tsitsiklis, Introduction to Linear Optimization, Athena Scientific Series in Optimization and Neural Computation,(Book 6), ISBN-10: 1886529191.
12. S. S. Rao, Engineering Optimization: Theory and Practice, Third Edition, Wiley Eastern Ltd.
13. W. F. Ramirez, Computational Methods for Process Simulation, Second Edition, Butterworth-Heinemann

Course Outcome:

After learning the course the students should be able to:

1. Use process models based on conservation principles and process data.
2. Simulate the chemical processes, different parts of the processes and unit operations.
3. Have an understanding of computational techniques to solve the process models.
4. Use economics to derive an objective function.
5. Use principles of engineering to develop equality and inequality constraints.
6. Get familiar with the preferred software packages and optimization techniques to solve linear programming and nonlinear programming problems.
7. Think about and use optimization as a tool in process design and operation.
8. Get proficient in the applications of optimization for optimizing important industrial processes.
9. Work on professional simulation software such as ASPEN PLUS, GAMS, HYSIS, CHEMCAD and MATLAB which will make them ready for industry.

List of Experiments:

Minimum 5 practicals are to be performed and a report is to be submitted for each of them stated in following sections below:-

Modeling:

Basic understanding of the software and the tools for the modeling purpose

- ➢ Solving one/two demo problems pre-defined in software for the understanding and getting use to the software.
- ➢ Modeling of ideal and non- ideal flow reactors like: CSTR, PFR, BATCH, etc.
- ➢ Modeling of unit operations like: Distillation, Evaporation, Extraction, etc.

Simulation:

Basic understanding of the software and the tools for the simulation purpose.

- ➢ Solving one/two demo problems pre-defined in software for the understanding and getting use to the software.
- ➢ Simulation of ideal and non- ideal flow reactors like: CSTR, PFR, BATCH, etc.
- ➢ Simulation of unit operations like: Distillation, Evaporation, Extraction, etc.

Optimization:

Basic understanding of the software and the tools for the optimization purpose.

- ➢ Solving one/two demo problems pre-defined in software for the understanding and getting use to the software.
- ➢ Optimization of ideal and non- ideal flow reactors like: CSTR, PFR, BATCH, etc.
- ➢ Optimization of unit operations like: Distillation, Evaporation, Extraction, etc.

Design based Problems (DP)/Open Ended Problem:

Design problem can be based on modeling, simulation or optimization as per the following:

- ➢ Modeling of any chemical engineering process system

- Solving one/two demo problems pre-defined in software for the understanding and getting use to the software.
- Optimization of ideal and non- ideal flow reactors like: CSTR, PFR, BATCH, etc.
- Optimization of unit operations like: Distillation, Evaporation, Extraction, etc.

List of Open Source Software/learning website:

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

Active Learning Assignments: Preparation of power-point slides, which include videos, animations, pictures, graphics for better understanding theory and practical work – The faculty will allocate chapters/ parts of chapters to groups of students so that the entire syllabus to be covered. The power-point slides should be put up on the web-site of the College/ Institute, along with the names of the students of the group, the name of the faculty, Department and College on the first slide. The best three works should submit to GTU.