GUJARAT TECHNOLOGICAL UNIVERSITY

Bachelor of Engineering
Subject Code: 3170513

Semester – VII

Subject Name: Process Modelling, Simulation and Optimization

Type of course: Professional Elective Course

Prerequisite: Basics kknowledge of unit operations, fundamental of process engineering, engineering mathematics and numerical computations.

Rationale: The Process Modelling, 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. The subject comprises of three parts: modelling, simulation and optimization. Modelling and simulation emphasize on the concept of modelling 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)	
3	0	2	4	70	30	30	20	150

Content:

Sr. No.	Content	Total Hrs
1	**Introduction :** Definition of Modelling, Simulation and Optimization, importance of modelling for simulation and optimization, comparison of design and simulation, scope and applications of modelling, simulation and optimization	3
2	**Modelling Aspects:** Definition of model, process model, deterministic and stochastic process, physical and mathematical modelling, classification of models, process to build a model, degrees of freedom analysis for model, empirical model, selecting functions to fit empirical data, Black-box model	4
3	**Mathematical Modelling of Chemical Engineering Systems:** Introduction, uses of mathematical models, scope of coverage, principles of	3

	formulation, fundamental laws, continuity equations, energy equations, equation of motion, transport equation, equation of state, equilibrium, kinetics.	
4	**Examples of Mathematical Models of Chemical Engineering systems:** flow tank, mixing tank, two heated tanks, PFR, CSTR, 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 with mass transfer, ideal binary distillation column, batch distillation with holdup, Solvent Extraction, gas adsorption	**6**
5	**Chemical Process Plant Simulation :** Steady state vs dynamic simulation, lumped system-partitioning equation, tearing equation, simultaneous equation, modular approaches & equation solving approaches, decomposition of networks, partition and tearing applied to process flow sheeting, reachability matrix, selection of property perdition method for simulation, Introduction to Various Professional Simulators and Equation Solver Software	**5**
6	**Basic Concepts of Optimization:** 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, continuity of function, 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.	**4**
7	**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 unidimensional search, polynomial approximation methods, how one-dimensional search is applied in a multidimensional problem, evaluation of unidimensional search methods, methods using function values only : Simplex search, Hooke-Jeees and Powell's method; methods that use first derivatives : Newton's method, Marquardt's method, Quasi-Newton methods.	**6**
8	**Linear Programming (LP) and Applications**: Formulation of linear programming models, LP in standard form, principles of simplex method, applications	**5**
9	**Constrained Optimization :** Lagrange's multiplier, Kuhn-Tucker conditions, transformation methods : penalty function, constrained direct search method: complex method, Quadratic approximation methods	**4**
10	**Application of Optimizations:** Examples and case studies 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, optimal location of coal-blending plant, optimization of Glycol-Ethylene Oxide process	**5**

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Suggested Specification table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
5	10	25	15	10	5

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. W. F. Ramirez, Computational Methods for Process Simulation, Second Edition, Butterworth Heinemann.
7. Edger, Himmelblau, Lasdon, Optimization of Chemical Processes, McGraw-Hill International Edition.
8. Gordon S. G. Beveridge and Rober S. Schechter, Optimization: Theory and Practice, McGrawHill Book Company.
9. M C Joshi and K M Moudgalya, Optimization: Theory and Practice, Narosa Publishing
10. S. S. Rao, Engineering Optimization: Theory and Practice, Third Edition, Wiley Eastern Ltd.
11. A. Ravindran, K.M. Ragsdell and G.V. Reklaitis, Engineering Optimization: Methods and Applications, Second Edition, Wiley

Course Outcomes:

After successful completion of the course, student will be able to

Sr. No.	CO statement	Marks % weightage
CO-1	Illustrate use of fundamental laws to develop model for Chemical engineering processes.	10

CO-2	Outline the scope of process optimization and its applications to chemical processes.	20
CO-3	Apply mathematical principles and techniques to solve the models for simulation.	20
CO-4	Analyse process plant simulation results using professional simulators.	25
CO-5	Formulate optimization problems and evaluate the solutions.	25

Suggested list of experiments to be performed (8 to 10 experiments are to be given)

Practical based on the syllabus topics to be planned. The list may include following experiments:

1. Familiarization to tools used for laboratory like Excel Spreadsheet, COCO/DWSIM (open source simulator and MATLAB/SCILAB (computation platform)
2. Solve single and multi-variable optimization problems in Excel Spreadsheet using solver
3. Solve Linear Programming problems in Excel Spreadsheet using solver
4. Estimate kinetic parameters of the reaction using batch reactor data
5. Plot ideal and non-ideal vapour liquid equilibrium (VLE) plots computing data using (i) ideal mixture assumption and (ii) using Van-Laar activity coefficient model
6. Determine composition of vapour and liquid streams in a flash distillation still using VLE data
7. Simulate continuous binary distillation column developing material and enthalpy balance in the column. Compute ideal number of places using optimal reflux ratio.
8. Simulate multicomponent distillation with reboiler and condenser.
9. Develop material and energy balance for adiabatic combustion of methane and simulate the effect of excess air on performance of combustion.
10. Develop simulation of shell and tube heat exchange and evaluate Rating / Design.
11. Develop design and optimization of single and multiple effect evaporator
12. Develop simulation of fed batch reactor to evaluate effect of initial volume and feed recipe on productivity and yield

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.
- Student can use DWSIM, COCO, ChemSep open source software for simulation study.
- Students can use Matlab, Scilab or GAMS software for the solution optimization problems.