GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Master of Engineering

Level: PG

Branch: Chemical Engineering

Subject Code: ME02030081

Subject Name: Advanced Optimization Techniques in Chemical Engineering

w. e. f. Academic Year:	2024-25
Semester:	2
Category of the Course:	Professional Elective Course

Prerequisite:	Concepts of Optimization of undergraduate level
Rationale:	Process Optimization is intended to teach students how to use optimization algorithms to improve the design and operation of chemical processes. This course emphasizes problem formulation; 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.

Course Outcome:

After Completion of the Course, Student will able to:

No	Course Outcomes
01	Understand optimization techniques to solve linear programming and nonlinear programming problems
02	Use optimization as a tool in process design and operation
03	Proficiency in the applications of optimization in chemical plants
04	Nontraditional optimization techniques application in other areas

Teaching and Examination Scheme:

Teaching Scheme(in Hours)			Total Credits L+T+ (PR/2)	Assessment Pattern and Marks				Total Marks
				Theory		Tutorial / Practical		
L	T	PR	C	ESE (E)	PA / CA (M)	PA/CA (I)	ESE (V)	
3	0	2	4	70	30	20	30	150

Course Content:

Unit No.	Content	No. of Hours	% of Weightage
1.	**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	**3**	**7**
2.	**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 Economic Objective Functions, The Time Value of Money in Objective Functions, Measures of Profitability	**6**	**13**
3.	**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**	**13**
4.	**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 method	**6**	**13**
5.	**Unconstrained Multivariable Optimization:** Methods Using Function Values Only, Methods That Use First Derivatives, Newton's Method, Quasi-Newton Methods	**5**	**12**
6.	**Linear Programming (LP) and Applications:** Geometry of Linear Programs, Basic Linear Programming Definitions and Results, Simplex Algorithm, Barrier Methods, Sensitivity Analysis, Linear Mixed Integer Programs, LP Software, A Transportation Problem Using the EXCEL Solver Spreadsheet Formulation, Network Flow and Assignment Problems	**7**	**16**
7.	**Non linear and mixed integer programming:** 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, Optimal pipe diameter etc.	**6**	**13**

8.	**Chemical reactor Design and operation:** Optimization of a Thermal Cracker Via Linear Programming, Optimal Design of an Ammonia Reactor Solution of an Alkylation Process by Sequential Quadratic Programming, Predicting Protein Folding, Optimization of Low-Pressure Chemical Vapor Deposition, Reactor for the Deposition of Thin Films Reaction Synthesis	**6**	**13**
	Total	**45**	**100**

Suggested Specification Table with Marks (Theory):

Distribution of Theory Marks					
R Level	**U Level**	**A Level**	**N Level**	**E Level**	**C Level**
7	12	35	10	6	0

Where R: Remember; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create (as per Revised Bloom's Taxonomy)

References/Suggested Learning Resources:

(a) Books:

1. Optimization of Chemical Processes by Edger, Himmelblau, Lasdon, McGraw-Hill International Edition.
2. Optimization: Theory and Practice by Gordon S. G. Beveridge and Rober S. Schechter, McGraw-Hill Book Company.
3. Optimization for Engineering Design by K. Deb, Prentice-Hall.
4. Optimization: Theory and Practice by MC Joshi and K M Moudgalya, Narosa Publishing.
5. Numerical Optimization by J Nocedal and S J Wright, Springer Verlag.
6. Introduction to Linear Optimization by Dimitris Bertsimas, John N. Tsitsiklis, John Tsitsiklis, Athena Scientific Series in Optimization and Neural Computation.

(b) Open source software and website:

1. Students can refer to video lectures available on the websites including NPTEL lecture series.
2. MS Excel, MATLAB, SCILAB, DWSIM

Suggested Course Practical List:

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. Simulate continuous binary distillation column developing material and enthalpy balance in the column. Compute ideal number of places using optimal reflux ratio.
7. Simulate multicomponent distillation with reboiler and condenser.
8. Develop material and energy balance for adiabatic combustion of methane and simulate the effect of excess air on performance of combustion
9. Develop simulation of shell and tube heat exchange and evaluate Rating / Design
10. Develop design and optimization of single and multiple effect evaporator

List of Laboratory/Learning Resources Required:

- Computer Lab

Suggested Project List:

- Minimize energy consumption while maximizing product purity using NLP or MILP.
- Use multi objective optimization for integrating solar wind or biomass energy.
- Apply genetic algorithms to identify optimal solvents for extraction process.
- Maximize yield and control particle size distribution using advanced techniques.
- Optimize the operating schedule for catalyst regeneration to minimize downtime.
- Apply dynamic optimization techniques to control temperature and concentration profiles.

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