FIRST SEMESTER 2022-2023
Course Handout (Part II)

Date: 16/08/2022

In addition to part I (General Handout for all courses appended to the time table) this portion gives further specific details regarding the course.

Course No: CHE G558

Course Title: Chemical Process Optimization

Instructor-in-charge: Dr. Arnab Dutta

Course Description: Introduction to Process Modelling and simulation, Fundamentals of analytical optimization. Survey of one dimensional line-search methods, and multi-dimensional unconstrained and constrained numerical optimization algorithms. Applications of linear programming, nonlinear programming, mixed integer linear/ nonlinear programming, and parameter estimation in chemical engineering. Feasible-path and infeasible-path techniques for chemical process flowsheet optimization, Evolutionary computation in Chemical Engineering.

Objective & Motivation:

The objective of this course is to introduce optimization techniques to students and discuss how to useoptimization algorithms to improve the design and operation of the chemical process industry. The coursewill be divided into three modules. The first module will emphasize the mathematical formulation of theoptimization problem. We will discuss how to develop an objective function of different types and theequality and inequality constraints.In the second module of the course, we will select a solution techniquethat is best suited for finding the maxima and minima of an objective function in single and multiplevariables

(both unconstrained and constrained). We will learn both linear and non-linear programming forthe particular type of objective function. Finally, in the third module, we will discuss some examples, casestudies, and evolutionary computation tools for solving the optimization problems associated withtheprocess industry.

Upon successful completion of this course, the student will be able to:

- **Identify an optimization problem**
- **Formulate objective function with decision variables and constraints**
- **Choose the appropriate method for the solution of the optimization problem**
- **Learn about applications of optimization in chemical engineering domain**
- **Get acquainted with MATLAB & MS-EXCEL to solve optimization problems**

Text Books:

T1: Optimization of Chemical Processes, T. F. Edgar, D. M. Himmelblau and L. S. Lasdon, 2nd

Edition,McGraw Hill, 2001.

T2: Engineering Optimization: Theory and Practice, S. S. Rao, 4th Edition, John Wiley & Sons, Inc, 2009

Course Plan:

Lec. No.	Learning Objectives	Topics to be covered	Resource
1	Introduction	▪ Get to know the students ▪ Understand students' notion about the subject ▪ Introduction to the course	--
2-3	What is Optimization& Why is it necessary?		Chapter: 1 (T1)
4-6	Formulation of Optimization problems	▪ Objective function ▪ Decision variables ▪ Constraints	Chapters:2-3 (T1), 1 (T2)

7-9	Fundamentals of analyticaloptimization	▪ Basic concepts: Continuity of functions ▪ Convex and concave functions ▪ Necessary &sufficient conditionsfor an extremum of anunconstrained function	Chapters: 4 (T1), 2 (T2)
10-15	Linear programming	▪ Geometry of linear programs ▪ Simplex algorithm ▪ Duality in linear programming ▪ Decomposition principle ▪ Sensitivity analysis	Chapters: 3-4 (T2), 7 (T1)
16	Hand-on session using MS-EXCEL & MATLAB for solving Linear Optimization Problems		
17-20	Nonlinear programming: One dimensional methods	▪ Elimination methods ▪ Interpolation methods	Chapter: 5 (T2)
21-25	Nonlinear programming: Unconstrained techniques	▪ Direct search methods ▪ Indirect search methods	Chapters: 6 (T2), 8(T1)
26-30	Nonlinear Programming: Constrained techniques	▪ Characteristics of a constrained problem ▪ Direct methods ▪ Indirect methods	Chapter: 7 (T2)
31	Hand-on session using MS-EXCEL & MATLAB for solving Nonlinear Optimization Problems		
32-34	Mixed Integer Programming		Chapters: 9 (T1), 10(T2)
35-37	Modern Methods of Optimization	▪ Particle Swarm Optimization (PSO) ▪ Genetic Algorithm (GA)	Chapter: 13 (T2)
38	Hand-on session using MATLAB for solving Optimization Problems using PSO & GA		
39-40	Introduction to Multi-objective Optimization		Chapter: 14 (T2)

1. **Evaluation Scheme:**

Component	Duration (minutes)	Weightage (%)	Date & Time	Remarks
Mid-Term	90	25	31/10 1.30 - 3.00PM	Open Book
Assignments: 2	--	30	TBA in the class	Nature of assignments will be discussed in the class
Project: 1	--	10	TBA in the class	Nature of project will be discussed in the class
Comprehensive Examination	180	35	19/12/2022 FN	Open Book

2. **Consultation Hour:** Will be announced in the class.

3. **Notices:** Notices concerning the course will be communicated via CMS.

4. **Make-up Policy:** Make-up will be granted only for genuine cases with valid justification and only with prior permission of Instructor-in-charge. Decision of the IC will be final.

5. **Academic Honesty and Integrity Policy:** Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

Arnab Dutta

Instructor-in-charge
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