**FIRST SEMESTER 2021-2022**
**Course Handout (Part II)**

Date: 05/08/2021

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.

1. **Objective & Motivation:**

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

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

**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<br>▪ Understand students' notion about the subject<br>▪ Introduction to the course | -- |
| 2-3 | What is Optimization & Why is it necessary? | | Chapter: 1 (T1) |
| 4-6 | Formulation of Optimization problems | ▪ Objective function<br>▪ Decision variables<br>▪ Constraints | Chapters: 2-3 (T1), 1 (T2) |
| 7-9 | Fundamentals of analytical optimization | ▪ Basic concepts: Continuity of functions<br><br>▪ Convex and concave functions<br><br>▪ Necessary & sufficient conditions | Chapters: 4 (T1), 2 (T2) |

| | | for an extremum of an unconstrained function | |
|---|---|---|---|
| 10-15 | Linear programming | ▪ Geometry of linear programs<br>▪ Simplex algorithm<br>▪ Duality in linear programming<br>▪ Decomposition principle<br>▪ Sensitivity analysis | Chapters: 3-4 (T2), 7 (T1) |
| 16-20 | Nonlinear programming: One dimensional methods | ▪ Elimination methods<br>▪ Interpolation methods | Chapter: 5 (T2) |
| 21-25 | Nonlinear programming: Unconstrained techniques | ▪ Direct search methods<br>▪ Indirect search methods | Chapters: 6 (T2), 8(T1) |
| 26-30 | Nonlinear Programming: Constrained techniques | ▪ Characteristics of a constrained problem<br>▪ Direct methods<br>▪ Indirect methods | Chapter: 7 (T2) |
| 31-33 | Mixed Integer Programming | | Chapters: 9 (T1), 10(T2) |
| 34-37 | Modern Methods of Optimization | ▪ Particle Swarm Optimization<br>▪ Genetic Algorithm | Chapter: 13 (T2) |
| 38-39 | Introduction to Multi-objective Optimization | | Chapter: 14 (T2) |

2. **Evaluation Scheme:**

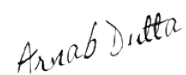| Component | Duration (minutes) | Weightage (%) | Date & Time | Remarks |
|---|---|---|---|---|
| Mid-Term | 90 | 30 | TBA Later | Open Book |
| Assignments: 2 | -- | 25 | TBA in the class | Nature of assignments will be discussed in the class |
| Project: 1 | -- | 10 | TBA in the class | Nature of project will be discussed in the class |
| Comprehensive Examination | 120 | 35 | TBA Later | Open Book |

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

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

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

6. **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**

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**Instructor-in-charge**
**CHE G558**