

Modelling Simulation and Optimization

1.1 Course Number: CH444

1.2 Contact Hours: 2-0-0 Credits: 06

1.3 Semester -Offered: 4th Year-even

1.4 Prerequisite: Not required

1.5 Syllabus Committee Member: Dr Amit Ranjan, Dr Vivek Kumar

2. **Objective:** The objective of course is to able the students to develop the mathematical modelling of chemical systems and processes as well as to provide the knowledge of algorithm and numerical simulation of mathematical models using MATLAB. The students will also be able to learn the parameter extraction and unconstrained & constrained optimization techniques.

3. Course Content

Unit-wise distribution of content and number of lectures

Unit	Topics	Sub-topics	Lectures
1	. Introduction	Mathematical modeling; Classification of models; Modeling procedure	2
2	Mechanistic Modeling	Review of transport based models and physicochemical principles of heat, mass and momentum transfer: Conservation principles, Constitutive relations, Boundary and initial conditions, Examples from heat conduction, mass transfer, fluid flow, and chemical reactor design; Population balance models: Examples from crystallization and flocculation. RTD (residence time distribution); Molecular scale models: Molecular dynamics and Monte Carlo methods	8
3	Empirical Modeling	Dimensionless representation of dimensional systems, Empirical model building. Scaling up	2
4	Simplification strategies	Decoupling equations, Simplifying geometries, Reducing number of variables, Lumping, Linearizing, Neglecting terms, Examples	2
5	Numerical Methods review (MATLAB based)	Quick review of the solution techniques to the following: Linear Systems, ODE, System of ODEs, PDEs (partial). Application on examples of modeling presented earlier	3

6	Optimization	Objective functions, convex functions, single variable single objective function optimization with examples, unconstrained vs constrained optimization, numerical methods: Interval halving, Fibonacci method, Newton Raphson method	5
7	Multivariable single objective functions	Unconstrained optimization, contour plots, numerical methods: NR, Line search, Steepest descent, Conjugate gradient method.	4
8	Constrained optimization	Geometric method, Lagrange multiplier method, Other specialized methods	2
Total			28

4. **Textbooks:**

1. Edgar, T. F. and Himmelblau, D. M.; "Optimization of Chemical Processes", McGraw-Hill Book Co., NY (2001)
2. Rao, S. S., "Engineering Optimization: Theory and Practice", New Age International (P) Ltd. Publishers, New Delhi (2013)
3. Luyben, W. L., "Process Modeling, Simulation and Control", McGraw-Hill Book Co. Inc., NY(1973)
4. Ramirez, W. "Computational Methods in Process Simulation", Butterworths Publishers,Oxford(1997)

5. **Outcome of the course**

At the end of this end, the students will have the knowledge of mathematical modelling and their solution using MATLAB. The students will also have the knowledge of regression and the multivariable optimization techniques.