

Modelling Simulation and Optimization

1.2 Course Number: CH443

1.3 Contact Hours: 3-0-0 Credits: 9

1.4 Semester -Offered: 4th Year-even

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

2. Objective: The objective of the course is to learn different mathematical modeling techniques and optimization methods.

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	5
3	Empirical Modeling	Dimensionless representation of dimensional systems, Empirical model building. Scaling up	3
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). Applying these methods to examples of modeling presented earlier	10
6	Parameter Extraction and statistical analysis of mathematical models	Curve fitting, Linear and Non-linear regression Some simulation tools with examples	6
7	Optimization	Objective functions, convex functions, single variable single objective function	4

		optimization with examples, unconstrained vs constrained optimization, numerical methods: Interval halving, Fibonacci method, Newton Raphson method	
8	Multivariable single objective functions	Unconstrained optimization, contour plots, numerical methods: NR, Line search, Steepest descent, Conjugate gradient method.	6
9	Constrained optimization	Geometric method, Lagrange multiplier method, Other specialized methods	2
Total			40

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:** The student will be able to know the basics of mathematical modeling techniques and optimization methods.