5ᵗʰSemester	RCH5D002	PROCESS SIMULATION & MODELLING	L-T-P 3-0-0	3 CREDITS

Module I: **(12 hr)**

Modelling Based on First Principles: Fundamentals of mathematical models and formulation – Continuity equation, Equation of motion, Transport equations, Energy equation, Equations of state, Equilibrium, Chemical kinetics and their applications; Lumped and distributed parameter models – Fluid systems, C.S.T.R. (single, series, isothermal, constant hold up, variable hold up, gas phase pressurized and non-isothermal), Single component vaporizer, Multi-component flash drum, Batch reactor, Reactor with mass transfer, Ideal binary distillation column, Batch distillation, Heat exchanger, etc.

Module II: **(7 hr)**

Optimization

Single variable optimization (Pointwise/exhaustive search and Gradient based search algorithms)

Multivariable optimization (Pointwise/exhaustive search and Gradient based search algorithms)

Non-traditional Optimization algorithms

➤ Probabilistic algorithm (Simulated annealing)
➤ Evolutionary search (Differential evolution algorithm).

Module III: **(10 hrs)**

Numerical Methods

Generalized concepts of vector space, linear dependence, and matrix norms, Linear and Nonlinear Algebraic Equation solution, Solution of differential equation (Euler's method, Runge-Kutta method, finite difference method, Orthogonal collocation method), Partial differential equation (elliptic, parabolic and hyperbolic PDEs, Dirichlet , Neumann and Robin boundary conditions, solution of PDEs' by method of lines using *Crank-Nicholson* method, finite difference method)

Module IV: **(8 hr)**

Simulation

1. Linearization and state space models
2. Model transformation using theory of approximation
3. Devising numerical Methods
➤ Information flow from process to information flow diagram,
➤ From information flow diagram to numerical form
➤ Recycles
4. Dynamic and Steady state simulation using solvers (like MATLAB ODE solver, ASPEN PLUS, and SIMULINK)

Books:

1. Process Modeling, Simulation, and Control for Chemical Engineers, 2nd ed. by W LLuyben, McGraw-Hill.
2. B. Roffel, B. Betlem, "*Process Dynamics & Control: Modeling for control and prediction*. John Wiley & Sons Ltd., 2006.
3. Numerical Methods for Engineers 4th Edition 2019 by Gupta, Santosh K, New Age International (P) Ltd Publishers
4. Process Plant Simulation, B V Babu, Oxford University Press
5. Engineering Optimization: Theory and Practice by S S Rao, New Age.

6. Kalyanmoy Deb, Optimization for Engineering Design: Algorithms and Examples, 2nd Edition, PHI, 2012.
7. Process Control: Modelling, Design and Simulation, 1st ed. by B W Bequette, PHI.

Digital learning resources:

1. Process Modelling and Simulation by Dr. V. K. Agrawal Department of Chemical Engineering, IIT Roorkee (Link: https://nptel.ac.in/courses/103/107/103107096/)
2. Advanced Numerical Analysis by Prof. Sachin C. Patwardhan, Department of Chemical, Engineering, IIT Bombay (Link: https://nptel.ac.in/courses/103/101/103101111/)