IV Year B.Tech. Chemical Engg.   I - Semester

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CH405 PROCESS MODELING AND SIMULATION

Course Description & Objectives:
To make the students understand physical systems in chemical engineering and to develop their mathematical models and solutions for these models. The students will also learn to use the commercial process simulators.

Course Outcomes:
1. *Understand the important physical phenomena from the problem statement.*
2. *Develop model equations for the given system.*
3. *Demonstrate the model solving ability for various processes/unit operations.*
4. *Demonstrate the ability to use a process simulation.*

UNIT I - Fundamentals
Mathematical models for chemical engineering systems, fundamentals, introduction to fundamental laws, examples of mathematical models of chemical engineering systems, constant volume CSTRS, two heated tanks.

UNIT II - Examples
Gas phase pressurized CSTR, non-isothermal CSTR, single component vaporizer, batch reactor, reactor with mass transfer, ideal binary distillation column, batch distillation with holdup.

UNIT III - Iterative Methods
Bisection, false position, Newton –Raphson, successive approximation method, comparison of iterative methods.
Solution of Linear Simultaneous Algebraic Equations: Computation of Eigen values and Eigen vectors, Gauss elimination method, Gauss-Jordan and Gauss-Seidel's method.

UNIT IV - Numerical Integration
Trapezoidal and Simpson's rules.
Numerical Solution of Differential Equations**:** Euler method, Runge-Kutta fourth order method, Milne predictor corrector method.
Interpolation**:** Lagrange interpolation, forward difference, backward difference and central difference interpolation methods, least square approximation of functions.

UNIT V - Computer Simulation Examples
Gravity flow tank, three CSTRs in series, binary distillation column, batch reactor, Non-isothermal CSTR, VLE dew point, bubble point calculations, countercurrent heat exchanger.

TEXT BOOKS
1. William L. Luyben, "Process Modeling, Simulation and Control for Chemical Engineers", 2nd ed., McGraw - Hill International, 1990.
2. Santosh.K. Gupta, "Numerical Methods in Engineering", 2nd ed., New Age International (P) Ltd., 2003.

REFERENCE BOOK
1. K.Balu and K.Padmanabhan, "Modeling and Analysis of Chemical Engineering Processes", IK International Private Limited, 2007.