PROCESS MODELING AND SIMULATIONS
ENCH 413

Lecture : 3 **Year : IV**
Tutorial : 2 **Part : I**
Practical : 1.5

Course Objectives:
The objective of this course is to introduce the fundamental concepts of process modeling and simulation, train students to build mathematical models, and identify simple and complex modeling approaches in chemical engineering. It enables students to incorporate modeling and simulation techniques to solve chemical engineering problems effectively.

1 Introduction to Process Modeling (4 hours)

1.1 Introduction to models and modeling
1.2 Introduction to MATLAB and modeling tools
1.3 Approaches to Modeling (first-principles, empirical, hybrid)
1.4 Classification of Models
1.5 Steady-State vs Dynamic System

2 Numerical Methods for Chemical Engineering Systems (6 Hours)

2.1 Numerical solutions for ODEs (Euler, Runge-Kutta methods)
2.2 Numerical solutions for PDEs (finite difference concept)
2.3 Numerical solutions for systems of linear equations
2.4 Numerical solutions for nonlinear equations (Newton–Raphson)
2.5 Numerical solutions for differential equation systems utilizing MATLAB inbuilt functions

3 General Models in Chemical Engineering Systems (7 Hours)

3.1 Mass balance model development
3.2 Energy balance model development
3.3 Momentum balance model development
3.4 Modeling of thermodynamic and physical properties
3.5 Model assumptions and boundary conditions

4 Flash Seperator Modeling (7 Hours)

4.1 Thermodynamic equilibrium concepts
4.2 Implementation of equilibrium relations
4.3 Development of simulation for a flash separator
4.4 MATLAB implementation and example case study

5 Distillation Modeling (7 Hours)

5.1 Concept of stagewise separation
5.2 Compartmental (stage) models for distillation
5.3 Equation of state models
5.4 Activity coefficient models
5.5 Simplified column simulation approach

6 Reactor Modeling (8 Hours)

6.1 Batch reactor modeling
6.2 Continuous stirred tank reactor (CSTR) modeling
6.3 Plug flow reactor (PFR) modeling
6.4 Mass and energy balance coupling
6.5 Numerical simulation of reactor performance

7 Chemical Flowsheet Simulation (8 Hours)

7.1 Concept of process flowsheet modeling
7.2 Sequential modular simulation strategy
7.3 Steady-state flowsheet example without recycle
7.4 Steady-state flowsheet example with recycle loop

Tutorial (30 hours)

1. Model selection and problem formulation for selected chemical processes.
2. Numerical methods for solving engineering equations manually.
3. Development of mass and energy balance models.
4. Mathematical modeling of chemical reactors.
5. Flash separator model formulation.
6. Distillation column model formulation.

Practical (15 hours)

1. Introduction to MATLAB/Python for engineering simulation.
2. Implementation of numerical methods in software.
3. Simulation of dynamic systems using ODE solvers.
4. Simulation of batch and CSTR reactor models.
5. Simulation of flash separator and VLE generation.
6. Simulation of distillation column performance.
7. Chemical process flowsheet simulation

Evaluation Scheme:

The questions will cover all the chapters in the syllabus. The evaluation scheme will be as follows:

Chapter	Hours	Mark distribution*
1 and 2	10	10
3	7	8

4	7	8
5	7	10
6	8	12
7	8	12
Total	**45**	**60**

References

1. Bungartz, H.-J., Zimmer, S., Buchholz, M., & Pflüger, D. (2013). Modeling and simulation: An application-oriented introduction. Springer Science & Business Media.
2. Ingham, J., Dunn, I. J., Heinzle, E., & Přenosil, J. E. (2007). Chemical engineering dynamics: An introduction to modelling and computer simulation (3rd ed.). Wiley-VCH.
3. Jana, A. K. (2011). Chemical process modelling and computer simulation (2nd ed.). PHI Learning.
4. Upreti, S. R. (2017). Process modeling and simulation for chemical engineers: Theory and practice. John Wiley & Sons.