Course Syllabus

Course No : **CHEG 305** (3 Credits)
Course Title : Modeling and Simulation in Chemical Engineering
Text Book : Verma, A.K., 2014. Process Modelling and Simulation in Chemical, Biochemical and Environmental Engineering. CRC Press, Boca Raton.

References:

1. Ingham, J., Dunn, I.J., Heinzle, E., Prenosil, J.E., Snape, J.B., 2007. Chemical Engineering Dynamics, Includes CD-ROM: An Introduction to Modelling and Computer Simulation, 3rd, Completely Revised Edition edition. ed. Wiley-VCH, Weinheim : Chichester.
2. Geankoplis, C.J., 1993. Transport Processes And Unit Operations. Third Edition. Prentice-Hall International.
3. Finlayson, B.A., 2014. Introduction to Chemical Engineering Computing, Second Edition, Wiley.
4. Python Book
5. Class note and print materials
6. Lab experiments

Course Objectives:

1. Acquaint the students with the concepts of modeling and simulation
2. Acquire knowledge about how to develop a model
3. Analyze and apply various simple and complex models in Chemical Engineering
4. Simulation of physical, chemical and biological processes

Course Plan:

Topics

Chapters	**Lecture hours**	**Textbook chapters**
Introduction to Modelling and Simulation: Chemical Processes, Simulation, Modelling;	2	1.1, 1.2, 1.3, 1.4
An Overview of Modelling and Simulation: Strategy for Simulation, Approaches for Model Development, Types of Models, Types of Equations in a Model and Solution Strategy, Sources of Equations, Simplifying Concepts;	10	2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7
Models Based on Simple Laws: Equation of State, Henry's Law, Newton's Law of Viscosity, Fourier's Law of Heat Conduction, Fick's First Law, Fick's Second Law, Film Model, Two-Film Theory, Arrhenius' Law, Adsorption Isotherms;	8	3.1, 3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8, 3.9, 3.10
Models Based on Laws of Conservation: Laws of Conservation of Momentum, Mass and Energy, Laminar Flow, Boundary Layers: Momentum, Thermal and Diffusional, Simple Models for Reactors and Bioreactors;	12	4.1, 4.2, 4.3, 4.7, 4.8
Population Balance Models and Discrete-Event Models: Stochastic Models, The Complex Nature of the Dispersed Phase, Population Balance Equation;	4	7.1, 7.2, 7.3
Artificial Neural Network–Based Models: Artificial Neural	5	8.1, 8.2, 8.3, 8.4, 8.5,

Networks, Development of ANN-Based Models, Applications of ANNs in Chemical Engineering, Advantages of ANN-Based Models, Limitations of ANN-Based Models;		8.7
Model Validation and Sensitivity Analysis: Objective of Model Validation, Model Validation Methodology, Sensitivity Analysis, Role of Sensitivity Analysis.	4	9.1, 9.2, 9.3, 9.5, 9.6
Total hours	45	

Lab Experiments

1. CSTRCOM
2. Population growth model
3. VARMOL
4. EOS models
5. Simple laws 1 (Adsorption models)
6. Simple laws 2,3, 4
7. Diffusion 1,2,3,4
8. Single tank mass balance
9. Tube diameter in PFR
10. Heterogenous stirred tank reactor
11. Ideal gas model
12. Bubble & dew point for binary mixture
13. ANN model
14. Sensitivity analysis
15. Numerical simulation of Navier-Stokes Equation + CFL condition
16. Openmodelica simulation
17. Miscellaneous experiments

Internal Evaluation (50 marks)

Subjective – 13 marks

Objective – 7 marks

Lab report – 10 marks

Mini-project (report + presentation) – 20 marks