First Semester 2015-2016
Course Handout (Part-II)

Date: 03/08/2015

In addition to Part I (General Handout for all courses appended to the Time Table), this portion gives further specific details regarding the course.

Course No. : **CHE F418**
Course Title : **Modeling and Simulation in Chemical Engineering**
Instructor-in-Charge : **Subhajit Majumder**

Course Description

The Modeling and Simulation of Chemical Engineering processes is a subject of major importance for the knowledge of unitary processes of transport and kinetics. Basically it deals with three aspects, namely; modeling of chemical engineering processes, parameter estimations and application of numerical methods for solution of models. In this course first chapter is devoted to introduction of the course and discusses the process modeling and need of simulation. Subsequently it follows the parameter estimation, tools of simulation, development of models, classification of models, unit models of unit process, models of mass transfer equipment, heat transfer equipment, reactors, and application of numerical methods for solutions of models.

Scope & Objective

Process simulation, tools of simulation, parameter estimation, models and classification of models, alternate classification of models, mathematical modeling based on transport phenomena, population balance, principles of probability and experimental data. Unit models of unit processes, detailed mathematical models of mass transfer equipment, heat transfer equipment, reactors, modular and equation-solving approaches in simulation, decomposition of network, convergence promotion.

Pre-requisites

Basic knowledge of Courses on Material & Energy Balance; Transport Phenomena and Numerical methods.

Text Books

TB Babu B.V., "Process Plant Simulation", 1st Ed., Oxford University Press, 2004.

Reference Books:

R1 Luyben W. L., "Process Modeling Simulation and Control for Chemical Engineers", 2nd Ed., McGraw Hill, 1990.
R2 Najim K., "Process Modeling and Control in Chemical Engineering", CRC, 1990.
R3 Aris R., "Mathematical Modeling, Vol. 1: A Chemical Engineering Perspective (Process System Engineering)", Academic Press, 1999.

Course Plan

Lecture No.	Learning Objectives	Topics to be covered	Reference Chap./Sec. (Text Book/ Reference Book)
1	Introduction	Introduction to process modeling and simulation, Process synthesis and process analysis, Process modeling, Deterministic vs stochastic processes	Ch. 1.1, 1.2 and Ch. 2.1 of TB
PART I (MODELING)			
2-3	Process Modeling	Physical modeling, Mathematical modeling, Chemical system modeling	Ch. 2.2, 2.3, 2.4 of TB
4-5		Fundamental laws	Ch. 2.2 of R1
6-7		Classification of Mathematical modeling	Ch. 3 of TB
8-12	Chemical System Modeling	Models in mass transfer operations: solvent extraction, CSTR, mixing tank, gas absorption, distillation	Ch. 4 of TB and Class notes
13-17		Models in heat transfer operations: conduction through hollow cylindrical pipe, heating of a liquid, heat loss through maturing tank, heat transfer through extended surfaces, heat transfer in tubular gas preheater	Ch. 5 of TB
18-21		Models in fluid flow operations: continuity equation, flow through packed bed column	Ch. 6.1 and 6.2 of TB
22-23		Models in reaction engineering: chemical reaction with diffusion in a tubular reactor, reactors in series	Ch. 7.1 and 7.4 of TB
PART II (SIMULATION)			
24-26	Modular Approaches and Equation-solving approach	Analysis vs design mode, precedence, disjoining, the SWS algorithm	Ch. 11 of TB
27-31	Decomposition of Networks	Algorithm based on Signal Flow Graph: Tearing algoriths, Barkley and Motard algorithm, Basic Tearing algorithm	Ch. 12.1 and 12.2 of TB
32-35		Algorithm based on Reduced Digraph: Kehat algorithm, M&H algorithm	Ch. 12.3 of TB
36-37	Convergence Promotion	Newton's method, Direct substitution and Quasi Newton methods	Ch. 13.1 of TB
38-40	Industrial Simulation Package	Aspen Plus, methodology of Aspen Plus usage for industrial case studies	Class notes/ Demonstration

Evaluation Scheme (Total Marks 200)

EC No.	Evaluation component (EC)	Duration (Minutes)	Weightage (%)	Date and time	Nature of component
1	Mid-Semester Test	90	30	7/10 2:00 - 3:30 PM	Closed Book
2	Surprise Tests[#]	-	20	-	Closed Book/ Open Book[*]
3	Assignment[$]	-	10	To be announced in the class in due course of time	Continuous Monitoring
4	Comprehensive Examination	180	40	7/12 FN	Closed Book

[#] Total **six surprise tests** will be conducted. Out of these, the performance in **best four** will be considered for final evaluation. Each surprise test will carry 10 marks. During surprise tests, students will be asked to solve problems and submit the answer sheet to the instructor.

[$]Conceptual problems/case studies will be given as Assignment.

*During open book evaluation, **only text book and class notes are allowed.** Xerox copies of any other materials are not allowed.

Chamber Consultation Hour: To be announced in the class.

Make-up policy: Make-up will be granted only when one attends more than 75% classes and has genuine reason(s) (medical ground only) for not appearing in the regular test. Proper proofs (medical certificate, prescription etc. from Medical Center) must be submitted along with Make-up application. **Prior permission of IC is compulsory**.

Notices: All notices concerning this course will be displayed on the Notice Board of Chemical Engineering Department and will also be available online on NALANDA Portal.

Instructor-in-charge
CHE F418
Email: subhajit@pilani.bits-pilani.ac.in