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

Date: 13/01/2016

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 : **Modelling and Simulation in Chemical Engineering**
Instructor-in-Charge : **Subhajit Majumder**

Course Description

The Modelling 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; modelling 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 modelling 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

This course is designed to have detailed understanding of process simulation, tools of simulation, parameter estimation, models and classification of models, alternate classification of models, mathematical modelling. The primary objective of the course is to formulate mathematical models for mass transfer, heat transfer, fluid flow operations and reaction engineering aspects. It also caters the role of simulations and simulators in industrial applications by covering in-depth knowledge of modular & equation-solving approaches in simulation, decomposition of network and 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	Learning outcome	Reference Chap./Sec. (Text Book/ Reference Book)
1	Introduction	Introduction to process modelling and simulation, Process synthesis and process analysis, Process modelling, Deterministic vs stochastic processes	Mathematical models and their necessities. Knowledge of simulation	Ch. 1.1, 1.2 and Ch. 2.1 of TB
PART I (MODELLING)				
2-3	Process Modelling	Physical modelling, Mathematical modelling, Chemical system modelling	Knowledge of Physical and Mathematical models, Modelling in Chemical Engineering	Ch. 2.2, 2.3, 2.4 of TB
4-5		Fundamental laws	Formulation of dynamic models with case studies based on mass, component, momentum and energy balances	Ch. 2.2 of R1
6-7		Classification of Mathematical modelling	Knowledge of Mathematical models (classification)	Ch. 3 of TB
8-11	Chemical System Modelling	Models in mass transfer operations: solvent extraction, CSTR, mixing tank, gas absorption, distillation	Formulation of models in mass transfer phenomena	Ch. 4 of TB and Class notes
12-18		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	Formulation of models in heat transfer	Ch. 5 of TB
19-20		Models in fluid flow operations: continuity equation, flow through packed bed column	Formulation of models selected fluid	Ch. 6.1 and 6.2 of TB

			flow operations	
21-22		Models in reaction engineering: chemical reaction with diffusion in a tubular reactor, reactors in series	Formulation of models in reaction engineering phenomena	Ch. 7.1 and 7.4 of TB
PART II (SIMULATION)				
23-25	Modular Approaches and Equation-solving approach	Analysis vs design mode, precedence, disjoining, the SWS algorithm	Role of simulation and simulators in industrial applications. Knowledge of sequential and modular approaches to process simulation	Ch. 11 of TB
26-27	Industrial Simulation Package	Aspen Plus, methodology of Aspen Plus usage for industrial case studies	Get acquainted with industrial process simulation package	Demonstration
28-30	Decomposition of Networks	Algorithm based on Signal Flow Graph: Tearing algorithms, Barkley and Motard algorithm, Basic Tearing algorithm	Knowledge of different decomposition algorithms to reduce the number of process streams	Ch. 12.1 and 12.2 of TB
31-34		Algorithm based on Reduced Digraph: Kehat algorithm, M&H algorithm		Ch. 12.3 of TB
35-37	Convergence Promotion	Newton's method, Direct substitution and Quasi Newton methods	Methodologies for physical and thermodynamic properties required for process plant simulation	Ch. 13.1 of TB
38-40	Specific Purpose Simulation	Selected industrial problems/ case studies	Application of different simulation algorithms in industries	Ch. 14 of TB (selected portions)

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	14/3 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	4/5 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.
Out of six surprise tests, **three** will be conducted before mid-semester examination.

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

*During open book evaluation, **only text book is allowed.** Class notes and 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 in case of genuine reason(s) (medical ground only) for not appearing in the regular tests **(Mid-Semester and Comprehensive Examinations)**. **Make-up will not be given for surprise tests.** 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
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