Second Semester 2020-2021
Course Handout

Date: 12/01/2021

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

Course No. : **CHE F418**
Course Title : **Modelling and Simulation in Chemical Engineering**
Instructor-in-Charge : **SRINIVAS APPARI**

1. 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.

2. 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.

3. Text Books

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

4. Reference Books:

R1 Luyben W. L., "Process Modeling Simulation and Control for Chemical Engineers", 2nd Ed., McGraw Hill, 1990.
R2 Jenson V G, Jeffreys G V, “Mathematical methods in chemical engineering”, Academic press, Elsevier, second Ed, 2015
R3 Aris R., "Mathematical Modeling, Vol. 1: A Chemical Engineering Perspective (Process System Engineering)", Academic Press, 1999.
R4 Husain, A., “Chemical Process Simulation”, Wiley Eastern, New Delhi, 1986.

5. Course Plan

Module No	Lecture session	Reference Chap./Sec. (Text Book/ Reference Book)	Learning outcome
1. Introduction	L. 1.1. Introduction to process modelling and simulation, Process synthesis and process analysis, Process modelling, Deterministic vs stochastic processes	Ch. 1.1, 1.2 and Ch. 2.1 of TB, R4	Understand the importance of mathematical modeling and simulations
2. Process Modelling	L. 2.1. Physical modeling and mathematical modeling	TB- Ch. 2.2 – 2.3, R4	Understand the modeling concepts
	L. 2.2. Chemical system modeling	TB- Ch. 2.4, R4	Understand the formulations and laws in modeling
	L. 2. 3. Fundamental laws: Total continuity and component continuity equations with examples	R1- Ch. 2.2, R4	Understand the mass and component balances for various situations
	L. 2. 4. Energy balance equations and momentum balance	R1- Ch. 2.2,	Able to perform the energy balance equations for CSTR and PFR
3. Classification of mathematical modeling	L. 3. 1. Variables concepts, classification based on state of the process and type of the process	TB- Ch. 3.1 to 3.3, R4	Understand the various variables and its classifications
	L. 3. 2. Boundary conditions and black box principle	L. Ch. 3.3 to 3.6, R4	Understand the importance of boundary conditions for solving the model
4. Chemical system modeling: Models in mass transfer operations	L. 4. 1. solvent extraction	TB- Ch. 4.1 – 4.2, R2	Able to perform the modeling of simple mass transfer operation systems

	L. 4. 2. CSTR modeling	TB- Ch. 4.5 to 4.6, R2	Able to perform the modeling of CSTR
	L. 4.3. Gas absorption modeling	TB- Ch. 4.9, R2	Able to perform the modeling of absorption system
	L. 4.4. Multi stage distillation modeling	TB- Ch. 4.10, R2	Able to perform the modeling of distillation column
5. Chemical systems modeling: Models in heat transfer	L. 5. 1. Steady state heat conduction through a hollow cylindrical pipe	TB- Ch. 5.1, R2	Able to formulate the conduction heat transfer of a cylindrical system
	L. 5. 2. Steam heating of a liquid	TB- Ch. 5.2, R2	Able to perform the modeling of heat transfer processes
	L. 5. 3. Heat loss through maturing tank	TB- Ch. 5.3, R2	
	L. 5. 4. Heat transfer through extended surfaces	TB- Ch. 5.5, R2	
	L. 5. 5. Temperature distribution in a transverse cooling fin of triangular cross section	TB- Ch. 5.6, R2	
	L. 5.6. heat transfer in tubular gas preheater	TB- Ch. 5.7, R2	
	L. 5. 7. Heat loss through pipe flanges	TB. Ch. 5.8, R2	
6. Chemical systems modeling: Fluid flow operations	L. 6. 1. Continuity equation for fluid flow	TB- Ch. 6.1, R2	Able to develop the continuity equation for a given system
	L. 6.2. Flow through a packed bed	TB- Ch. 6.2, R2	Understand the modeling of packed systems
7. Chemical systems modeling: Reaction engineering	L. 7.1. Reaction with diffusion in a tubular reactor& Non Isothermal reactors	TB- Ch. 7.1, R2	Able to perform the modeling of non ideal reactor
	L. 7.2. Reaction with heat transfer in a packed bed reactor	TB- Ch. 7.2, R2	Able to perform the non-isothermal modeling of PFR

	L. 7.3. Gas absorption with reaction	TB- Ch. 7.3, R2	Able to perform the modeling of absorption with reaction
	L. 7.4. Reactors in series- I- Isothermal	TB- Ch. 7.4, R2	Able to perform the modeling of CSTRs in series
	L. 7.5. Reactors in series- II- Non isothermal	TB- Ch. 7.5, R2	Able to perform the modeling of CSTRs in series with multiple reactions
8. Modular approaches and equation solving	L. 8.1. Modular approaches to process simulation	TB- Ch. 11.1, R4	Able to simulate the various equations
	L. 8.2. Equation solving approach: order of equation sets	TB- Ch. 11.2, R4	Able to identify the ordering and disjoining the equations
	L. 8.3. Tearing and SWS algorithm	TB- Ch. 11.2, R4, R4	Able to perform the tearing and equations and SWS algorithm
9. Decomposition of networks	L. 9.1. Tearing algorithm, Algorithm based signal flow graph	TB- Ch. 12.1, R4	Able to understand the various algorithms for solving equations
	L. 9.2. Barkley and Motard algorithm	TB- Ch. 12.2, R4	Able to understand the various algorithms for solving equations
	L. 9.3. The basic tearing algorithm	TB- Ch. 12.2, R4	Able to understand tearing algorithm for solving equations
	L. 9.4. Kehat and Shacham algorithm	TB- Ch. 12.3, R4	Able to understand the Kehat and Shacham algorithms for solving equations

	L. 9.5. M & H algorithm	TB- Ch. 12.3, R4	Able to understand M &H algorithm for solving equations
10. Convergence promotion and physical and thermodynamic properties	L. 10.1. Newton's method, Direct substitution method, wegstein method	TB- Ch. 13.1	Able to select the suitable method to solve the set of equations
	L. 10.2. Eigen value methods, Quasi newton method	TB- ch. 13.1	Able to select the suitable method to solve the set of equations
	L. 10.3. Physical and thermodynamic properties	TB- Ch. 13.2	Understand the sources to get the data
11. Specific purpose simulation and dynamic simulation (carried out these simulations on DETCCHEM/ COMSOL? AspenHysis)	L. 11.1. Auto thermal ammonia synthesis reactor (	TB- Ch. 14.1, R4	Understand the modeling and simulation of a ammonia synthesis reactor
	L. 11. 2. Thermal cracking operation	TB- Ch. 14.2, R4	Understand the modeling and simulation of a thermal cracker
	L. 11.3. Design of shell and tube heat exchanger	TB- Ch. 14.3, R4	Understand the modeling and simulation of a shell and tube heat exchanger

6. Evaluation Scheme

EC No.	Evaluation component (EC)	Duration (Minutes)	Weightage (%)	Date and time	Nature of component
1	Mid-Semester Test	90	30		Close and/ or Open Book
2	Quiz tests[#]	-	15	-	Close / Open Book
3	Project[&]	-	10		Open book
4	Assignments (2)	-	05		Open book
5	Comprehensive Examination	180	40		Close and/ or Open Book

[#] Total **FIVE quiz tests** will be conducted. Out of these, the performance in **best THREE** will be considered for final evaluation.

[&]Project will be on modeling of chemical engineering systems using coding/ commercial/ open source softwares.

Important:

1. Chamber consultation hour: It will be announced in the class. Prior appointment via email or discussion in class is encouraged.
2. The notices, if any, concerning the course will be displayed on the Google Classroom/Nalanda only.
3. Make-up will be granted for genuine cases only. Proper certificate from authenticated doctor, say from the BITS Medical Center, must accompany make-up application (only prescription or vouchers for medicines will not be sufficient). Prior permission of IC is compulsory. No make- up will be granted for the tutorial tests.

Instructor-in-charge
CHE F418