Birla Institute of Technology & Science, Pilani
Hyderabad Campus

SECOND SEMESTER 2021-2022

Course Handout Part II

Date: 15-1-2022

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 : *Prof. Vikranth Kumar Surasani*

Scope and Objective of the Course:

Modeling and Simulation of Chemical Engineering processes has attracted the attention many scientists and engineers for many decades. It helps in understanding the dynamic behavior of the chemical processes is important from both process design and process control perspective. The prime objective of this course is to provide a more comprehensive treatment of process modeling, analysis and simulation of the dynamic chemical systems.

The topics that covering in this course is not covered in any traditional text books. Modeling and Simulation should be connected with Numerical Techniques. Implementation of Numerical techniques requires a programming language. In this Course, Programming using MATLAB & ANSYS will be taught. The generic modeling of the dynamic chemical systems will be taught using first principles as well as the Numerical Techniques that can be used to simulate the dynamics of the chemical processes.

Textbooks:

T1. Bruce A. Finlayson (2006), "Introduction to Chemical Engineering Computing", Wiley.

T2. Steven C. Chapra and Raymond P. Canale, "Numerical Methods for Engineers" Sixth Edition, McGraw Hill Education (India) Private Limited, New Delhi.

Reference books

R1. B. Wayne Bequette, "Process Dynamics Modeling, Analysis, and Simulation," Prentice-Hall-International, Inc., 1998.

R2. Rutherford Aris, "Mathematical Modeling: A Chemical Engineers' Perspective", Volume 1, Academic Press.

R3. Bird, Stewart and Lightfoot, 'Transport Phenomena', John Wiley & Sons, 2002, 2nd edition.

R4. Stefan J. Capmann, "Matlab Programming for Engineers", 4th Ed. Cengage Learning.

R5. Christie J. Geankoplis, 'Transport Processes and Unit Operations', Prentice Hall International, Inc., 1993, 3rd edition.

R6. Fogler, H. S. (1992). Elements of chemical reaction engineering, Prentice-Hall.

R7. Ansys Manuals

R8. P. Balbuena, K.E. Gubbins, Fluid Phase Equilib. 76 (1992) 21–35,
C. Lastoskie, K.E. Gubbins, N. Quirke, Langmuir 9 (1993) 2693–2702
A. Sengupta et al., Mol. Phys. 112 (2014),
J.R. Errington, Phys. Rev. E 67 (2003),
A. Sengupta and J. Adhikari, Chem. Phys. 469 – 470 (2016), 16 – 24
A. Sengupta and J. Adhikari, J. Mol. Liq. 221 (2016), 1184 – 1196

Course Plan:

Lecture No.	Learning objectives	Topics to be covered	Chapter in the Text Book
1-3	MATLAB Programming	Variable Types; Built in functions; Matrix operations	T1: Appendix B /R4: Ch. 2-6
		Plot tools;	
		Writing functions;	
		Control structures;	
		Managing variables;	
4-10	Numerical Techniques	Solution to System of Algebraic Equations: Direct Methods	T1, R1 and R2
		Solution to System of Algebraic Equations: Iterative Methods	
		Solution to System of Non-linear Algebraic Equations:	
		Solution to System of Ordinary Differential Equations (ODEs)	
		Explicit and Implicit Methods	
		R-K Methods	
11-16	Modeling and Simulation of Ideal Reactors	Simulations of Ideal Reactors: Batch Reactor	T1, R1 and R2
		Simulations of Ideal Reactors: CSTR	
		Simulations of Ideal Reactors: Plug Flow Reactor (PFR)	
		Simulations Non-isothermal Reactors	
17-28	Modeling of Chemical Engineering Systems	Mixing problems, Catalyst problems	T1, R2, R3, R5, and R6
		Fluidized bed and packed bed reactors, Dispersive Flow Problems	
		Slurry reactors. Moving boundary problems,	
		Prilling Tower problem, Pebble Heater.	
		Hydro-dynamic boundary layer and thermal boundary layer model development,.	
		Multistage Extraction, Multistage Distillation, Evaporators	
		Model development for dialysis and few membrane processes,	
25-29	Modelling and Special Topics	Multiphase flow in porous media. Drying of capillary porous media, O_2 & H_2O flow in PTL & CO2 Sequestration	R3, R5 and R8
30-40	Modeling Turbulence with ANSYS CFD	Introduction to Turbulence	Ansys Manuals
		Geometry & Meshing techniques	
		Simulation of turbulent combustion problems	

Evaluation Scheme:

Component	Duration	Weightage (%)	Date & Time	Nature of Component
Midsem Test	90 min	30	12/03 9.00am to10.30am	(15%) CB+(15%) OB (Require MATLAB)
Class Tests/Submissions (min 4)		15		CB (Require MATLAB and/ ANSYS)
Project		15		OB (Require MATLAB and/ ANSYS)
Comprehensive Exam	2 hours	40	11/05 FN	(40% OB) (Require MATLAB and/ ANSYS)

Academic Honesty and Integrity Policy: Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable

Chamber Consultation Hour: To be announced in the class.

Notices: All notices concerning this course will be displayed on the Chemical Engineering Notice Boards and CMS portal.

Make-up Policy: Make-up is granted only for genuine cases with valid justification and with prior permission of Instructor-in-charge.

INSTRUCTOR-IN-CHARGE