



## Birla Institute of Technology & Science, Pilani

Hyderabad Campus

### SECOND SEMESTER 2019-2020

#### Course Handout Part II

Date: 06-1-2020

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	: Dr. Angan Sengupta
Instructor(s)	: Dr. 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. Fogler, H. S. (1992). "Elements of chemical reaction engineering", Prentice-Hall.
- T2. Bird, Stewart and Lightfoot, 'Transport Phenomena', John Wiley & Sons, 2002, 2<sup>nd</sup> edition.

#### 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. Steven C. Chapra and Raymond P. Canale, "Numerical Methods for Engineers" Sixth Edition, McGraw Hill Education (India) Private Limited, New Delhi.
- R4. Stefan J. Capmann, "Matlab Programming for Engineers", 4<sup>th</sup> Ed. Cengage Learning.
- R5. Christie J. Geankoplis, 'Transport Processes and Unit Operations', Prentice Hall International, Inc., 1993, 3<sup>rd</sup> edition.
- R6. Bruce A. Finlayson (2006), "Introduction to Chemical Engineering Computing", Wiley.
- 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
1-6	Modelling and Simulation of Reactors	Introduction to modelling & simulations pertinent to present day in industry and research	T1, R1 and R2
		Mixing problems, Batch Reactor, CSTR, Plug Flow Reactor (PFR)	
		Dashpot model, Bioreactor modelling	
		Non-isothermal Reactors	
7-24	Modelling and Simulation of Chemical Engineering Systems	Stability and multiplicity, Cholette's model, Fluidized bed and packed bed reactors, Dispersive Flow Problems, Catalyst problems	Class notes, T1, T2, R2, R5 and R6
		Prilling tower problem, Pebble Heater	
		Slurry reactors, Moving boundary problems	
		Hydro-dynamic boundary layer and thermal boundary layer model development.	
		Multistage Extraction, Multistage Distillation, Evaporators	
		Model development for dialysis and few membrane processes	
25-35	Modelling and Simulation on Recent Special Topics	Determining independent and limiting reactions using simulation approach	Class notes and R8
		Predator-prey population model, Simple weather forecasting model, Introduction to Monte Carlo Simulations of bulk system and in porous media and Molecular Dynamics	
36-41	Modelling 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
Mid-sem Test	90 min	25	6/3 1.30 -3.00 PM	Closed Book (Require MATLAB and/ ANSYS)
Class Tests/Submissions	Continuous Evaluation	10	Surprise	Closed Book/ Open Book (Require MATLAB and/ ANSYS)
Project	Continuous Evaluation	30	TBA	Open Book (Require MATLAB and/ ANSYS)
Comprehensive Exam	3 hours	35	13/05 FN	Closed Book (Require MATLAB and/ ANSYS)

**Closed Book Test:** No reference materials of any kind will be permitted inside the exam hall.

**Open Book Exam:** Use of any text/ reference books are permitted. Loose sheets will not be permitted. Computers/mobile of any kind will not be allowed inside the exam hall. No exchange of any material will be allowed.

**Project Evaluation:** Mid and end term evaluations based on reports, viva/ presentation. Project done as a part of thesis or DOP/SOP/LOP will not be considered for evaluation.

**Chamber Consultation Hour:** To be announced in the class.



**Notices:** All notices concerning this course will be announced in Class or will be displayed on the Chemical Engineering Notice Boards or on the CMS portal.

**Make-up Policy:** Make-up for the Mid and End term exams may be granted with prior permission from Instructor-in-charge only for candidates having minimum 80% attendance or for any genuine case (certificate from an authenticated doctor from the Medical Center must accompany the make-up application. Only prescription or vouchers for medicines will not be sufficient). No make-up for Class tests/ submissions and project evaluation.

**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.

**INSTRUCTOR-IN-CHARGE**

