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**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, 2nd 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”, 4th Ed. Cengage Learning.

**R5.** Christie J. Geankoplis, ‘Transport Processes and Unit Operations’, Prentice Hall International, Inc.,

1993, 3rd 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:**

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| **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 |
| Determining independent and limiting reactions using simulation approach |
| 25-35 | Modelling and Simulation on Recent Special Topics | Predator-prey population model, Simple weather forecasting model, Introduction to Monte Carlo Simulations of bulk system and in porous media and Molecular Dynamics | Class notes and R8 |
| 36-41 | Modelling Turbulence with ANSYS CFD | Introduction to Turbulence | Ansys Manuals |
| Geometry & Meshing techniques |
| Simulation of turbulent combustion problems |

**Evaluation Scheme:**

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| **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**