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**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:**

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| --- | --- | --- | --- |
| **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, O2 & H2O 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:**

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| **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**