Birla Institute of Technology & Science, Pilani
Hyderabad Campus

ACADEMIC-GRADUATE STUDIES AND RESEARCH DIVISION

FIRST SEMESTER 2023-2024

Course Handout Part II

Date: 01-08-2023

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 G523***
Course Title	:	**Mathematical Methods in Chemical Engineering**
Instructor-in-Charge	:	**Dr. Afkham Mir and Dr. Balaji Krishnamurthy (IC)**

Scope and Objective of the Course:

The two main tasks facing engineers and scientists in chemical industry are (1) the operation and optimization of existing processes and (2) the design of new or improved ones. In the first task, information about the particular process under consideration and its qualitative aspects and criteria must be quantified. The basic variables and parameters of the relationships which describe the individual parts of the process must be worked out and the individual parts of the process must be combined. The Mathematical models play very important role in this respect. For the second task mathematical models help in applying existing processes to new or modified plants and in the definition of safer, more economically viable operating conditions. Data for the construction of new plants cannot be obtained from an operating process by running it to its technical limits; this entails a high degree of risk. In contrast, a mathematical model of a process is easy to manipulate. Unusual operating conditions can easily be simulated. The process or plant can even be modeled under hazardous conditions to define the limits of operating parameters or risk areas. Therefore, Mathematical Modeling and Simulation in Chemical Engineering processes has attracted the attention many scientists and engineers for many decades.

The prime objective of this course is to provide a more comprehensive treatment of process modeling, analysis and simulation of the dynamic chemical systems. First we would be focusing on modeling and simulation on the various chemical engineering processes based on first principles. Second, Mathematical Methods to model and simulate the various processes using Numerical Techniques. Students will be given a mini-projects to apply mathematical concepts and to simulate the chemical processes.

Learning Outcomes:

1. Understanding the modeling concepts of simple to complex chemical/biochemical processes.
2. Ability to write programs in MATLAB for simulating the chemical engineering processes.
3. Course is the basic foundation to advanced topic such as Optimization & Control theory

Textbooks:

T1. Steven C. Chapra and Raymond P. Canale, “Numerical Methods for Engineers” , Sixth Edition, McGraw Hill Education (India) Private Limited, New Delhi.

T2. S. Pushpavanam, “Mathematical Methods in Chemical Engineering,” Prentice-Hall-India, 1998.

Reference books

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

R1. Stefan J. Capmann, "Matlab Programming for Engineers", 4th Ed. Cengage Learning.

R3 Fogler, H. S. (1992). Elements of chemical reaction engineering, Prentice-Hall.

R4. Fromment G.F. and Bischoff K.B., Chemical Reactor Analysis and Design, John Wiley 1994.

R5. Bruce A. Finlayson, Introduction to Chemical Engineering Computing, 2nd Edition, Wiley

R6. Binay K. Dutta, Mathematical methods in Chemical and Biological Engineering, CRC press, 1st Edition.

Course Plan:

Lecture/Practical No.	Learning objectives	Topics to be covered	Chapter in the Text Book
L. 1-2	Introduction to Modeling & Simulation	Introduction to the course; Concept of simple mathematical model and conservation laws; Role of programming and software.	T1: Ch. 1 & 2
L. 3-12	Process Modeling	Introduction; Systems: Balance Equations	T2: Ch 1 / R1: Ch 1
		Material Balances and Constitutive Relations	T2: Ch 4 / R1: Ch 2
		Material and Energy Balances	
		Distributed Parameter Systems	
		General form of Dynamic Models	
L. 13-14	Numerical Techniques	System of Linear Algebraic Equation	T1: PART III
L. 15-18		Solution to Ordinary Differential Equations --Initial Valued Problem	T1: PART VII
L. 19-20		Solution Ordinary Differential Equations --Boundary Valued Problem	
L. 21-23		Least Square Regression	T1: Ch. 17
L. 24-25	Linear System Analysis	State Space Models	T2. Ch. 9 R1. Sec. III
L. 26-28		Linearization of Non-linear Models	
L. 29-31		Solution of general state-space form, Eigen value & Eigen Vector	
L. 32-33		Solving linear n^{th} order ODEs	
L. 34-35		Introduction to Laplace transforms	
L. 36-37		Analysis of First & Higher order Systems	
L. 38-41		Block Diagrams	
L. 41-43	Nonlinear System Analysis	Phase-Plane Analysis.	T1. Chap 10-12 R1. Sec. IV
		Introduction to Nonlinear dynamics	
		Bifurcation behavior for single Reactive Transport in Porous Media	
		Introduction to Population Balance modeling	
		Modeling of Exothermic CSTR	

Practical Plan

Lecture/Practical No.	Learning objectives	Topics to be covered
P. 1-2	Matlab/ExcelProgramming	Variable Types; Built in functions; Plot tools; Writing functions; Control structures; Managing variables; Matrix operations;
P. 3-4	Matlab/Excel Programming	Matlab Programming
P. 5	Linear Algebraic equations	Solution to Linear Algebraic Equations using Matlab/Excel
L. 15-20	ODEs	ODE, Explicit Methods; R-K methods
		Implicit method
		Boundary Value problems
P. 6	ODEs	Solution to Sys. of ODEs using Matlab
P. 7-8	PDEs	Solution to Sys. of PDEs using Matlab PDE Tool box
P. 9 & 10	Linear system Analysis	Matlab Step function & Initial function.
P.11-12	Linear system Analysis	Matlab Simulink module for stability analysis

Evaluation Scheme:

Component	Duration	Weightage (%)	Date & Time	Nature of Component
Mid Term	90 minutes	25%	10/10 - 11.30 - 1.00PM	5% CB/20% OB
Projects	--------	30%		OB
Assignments		10%		OB
Comprehensive	3 hours	35%	09/12 FN	10% CB/25% OB

Chamber Consultation Hour: Announced in the class

Notices: Display will be on the Chemical Engineering Group notice board and CMS.

Make-up Policy: Granted for genuine cases only. Certificate from authenticated doctor from the Medical Center must accompany make-up application (*only prescription or vouchers for medicines will not be sufficient*). Prior permission of IC is compulsory.

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
CHE G523