



Birla Institute of Technology & Science, Pilani
Hyderabad Campus

FIRST SEMESTER 2019-2020

Course Handout Part II

Date: 01-08-2019

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. Angan Sengupta

Scope and Objective of the Course:

The two main tasks facing engineers and scientists in the 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 a 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 modelled under hazardous conditions to define the limits of operating parameters or risk areas. Therefore, Mathematical Modelling and Simulation in Chemical Engineering processes has attracted the attention of many scientists and engineers for many decades.

The prime objective of this course is to provide a more comprehensive treatment of process modelling, analysis, and simulation of the dynamic chemical systems. First, we would be focusing on modelling 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 modelling concepts of simple to complex chemical/biochemical processes.
2. Ability to write programs in MATLAB for simulating the chemical engineering processes.
3. The course is the basic foundation for the 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. Gilbert Strang, “Introduction to Linear Algebra”, Fifth Edition, Wellesley-Cambridge Press.

Reference books

- R1. S. Pushpavanam, “Mathematical Methods in Chemical Engineering,” Prentice-Hall-India, 1998.
- R2. Fogler, H. S. (1992). Elements of chemical reaction engineering, Prentice-Hall.
- R3. Fromment G.F. and Bischoff K.B., Chemical Reactor Analysis and Design, John Wiley 1994.
- R4. Bruce A. Finlayson, Introduction to Chemical Engineering Computing, 2nd Edition, Wiley.
- R5. Stefan J. Capmann, “Matlab Programming for Engineers”, 4th Ed. Cengage Learning.

Course Plan:

Self Study: Taylor Series, Maclaurin Series and Basics on Matrices

Lecture No.	Learning objectives	Topics to be covered	Chapter in the Text Book
1-5	Fundamentals of Vector Spaces	Introduction to course, Vector spaces, Subspaces, Normed Linear Spaces and Banach Spaces, Induced Matrix Norms, Inner Product spaces and Hilbert Spaces, Gram-Schmidt Procedure, Projection Theorem.	T2, R1
6-13	Problem Discretization using Approximation Theory	Unified Problem Representation, Polynomial Approximation, Discretization using Taylor Series Approximation, Discretization using Polynomial Interpolation, Least Square Approximations, Errors in Discretization and Computations, Necessary and Sufficient Conditions for Unconstrained Optimality.	T2, R4
14-21	Linear Algebraic System	Introduction to the formation of Coupled Linear Model Equations for simple Chemical Engineering Systems, Search for the Existence of Solutions, Solving Techniques: Direct methods & Iterative methods , Matrix Conditioning and Solution Behaviour, Matrix Norms, Convergence Criteria for Iterative methods, Solving Chemical Engineering related Linear Model Equations.	T1, T2, R1, R4
22-28	Nonlinear Algebraic System	Introduction to Nonlinear Model Equations in Chemical Engineering, Solving Techniques: Method of Successive Substitutions, Newton Raphson Method and its Variants, Solutions	T1, R1 – R4



		of Nonlinear Model Equations using Optimization , Condition Number of Nonlinear Model Equations, Existence of Solutions, Convergence Criteria for Iterative methods.	
29-35	ODEs (IVP& BVP)	Introduction to various Chemical Engineering related ODEs, Basic Concepts, Methods based on Taylor Series Expansion to solve ODE-IVP, Convergence Analysis and Selection of Integration Interval, Solution of ODE-BVP using Finite Difference method and Shooting method.	T1, R1 – R4
36-38	PDEs	Introduction to various Chemical Engineering related PDEs, Types of PDEs and Boundary Conditions, Solution technique using Finite Difference method.	T1, R1 – R4
39-42	Multivariate Regression& Mathematical Modelling in Chemical Engineering	Model Parameter Estimation, Multivariate Linear Regression, Nonlinearity in Parameter Models, Types of Mathematical Models, Steps in Mathematical Model Formulation, Overview to Simulation Algorithm of Model Equations	T1, R4

Practical Plan:

Practical No.	Learning objectives	Topics to be covered
1	MatLab Introduction	Variable Types, Built in functions, Plot tools, Writing functions, Control structures, Managing variables, Matrix operations.
2-4	Linear Algebraic Equations	MatLab Coding to Direct and Iterative methods.
5-7	Nonlinear Algebraic Equations	MatLab Coding to Newton Raphson for Single and Coupled Equations and Coding of Newton Raphson Variants.
8-11	ODEs (IVP & BVP) and PDEs	MatLab Coding to Euler's method (Implicit & Explicit), class of Runge-Kutta methods, Finite Difference and Orthogonal Collocation methods.
12	Curve Fitting	MatLab Coding to Least Square method and using MatLab Curve Fitting tool.

Evaluation Scheme:

Component	Duration	Weightage (%)	Date & Time	Nature of Component
Midterm	90 mins.	30	30/9 (1:30 pm to	CB & Require MATLAB



			3:00 pm)	
Comprehensive	3 hrs.	30	5/12 (9:00 am to 12:00 noon)	CB & Require MATLAB
Practical Tests	To be decided	20	By I.C.	OB & Require MATLAB
Surprise Quizzes/ Class Assignments	Continuous Evaluation	20	By. I.C.	OB

Closed Book Test: No reference materials (if not prescribed otherwise during the course) 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.

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: Tuesday 5:00pm to 6:00pm in D-216.

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

Make-up Policy: Make-up for the test/ quizzes/ assignments 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 Centre must accompany the make-up application. Only prescription or vouchers for medicines will not be sufficient).

Dr. Angan Sengupta
INSTRUCTOR-IN-CHARGE

