BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI
HYDERABAD CAMPUS
INSTRUCTION DIVISION
First Semester 2016-2017
Course Handout (Part-II)

Date: 01/08/2016

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 G 523
Course Title: Mathematical Methods in Chemical Engineering
Instructor-in-Charge: Dr. Vikranth Kumar Surasani

1. Scope & Objective:

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. The course will introduce to various Matlab, and ANSYS for simulating the chemical engineering processes. Subsequently, it follows the modeling of the special cases from the simple to complex chemical/biochemical process engineering systems. Students will be given a mini-projects to apply mathematical concepts and to simulate the chemical processes.

2. Text and Journals Books:

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.

3. 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. (Available from Books 24x7)

R4 Fogler, H. S. (1992). Elements of chemical reaction engineering, Prentice-Hall.

R5. Froment G.F. and Bischoff K.B., Chemical Reactor Analysis and Design, John Wiley 1994.

R6. Bruce A. Finlayson, Introduction to Chemical Engineering Computing, 2nd Edition, Wiley

4. Journals

1. Lichtner, P. C. (1996). Continuum formulation of multicomponent-multiphase reactive transport. Reactive transport in porous media. P. C. Lichtner, C. I. Steefel and E. H. Oelkers. Washington, D. C., Mineralogical society of America. **34:** 1-81.
2. Surasani, V. K. (2008). A Non-isothermal Pore Network Drying Model, Docupoint-Verlag.
3. Surasani, V. K., F. Kretschmer, et al.(2011) "Biomass Combustion in a Fluidized-Bed System: An Integrated Model for Dynamic Plant Simulations." Industrial & Engineering Chemistry Research **50**(17): 9936-9943.
4. Surasani, V. K., L. Li, et al. (2014) "Bioclogging and Permeability Alteration by L. mesenteroides in a Sandstone Reservoir: A Reactive Transport Modeling Study." Energy & Fuels **27**(11): 6538-6551.
5. Surasani, V. K., T. Metzger, et al. (2008). "Consideration of heat transfer in pore network modelling of convective drying." International Journal of Heat and Mass Transfer **51**(9–10): 2506-2518.
6. Surasani V. K. (2005), "Isothermal and Non-isothermal Analysis of Diffusion Process in Inorganic Ceramic Membranes", Master Thesis Dissertation, Otto-von-Guericke University Magdeburg, Germany.

5. Course Plan:

Lecture No.	Learning Objectives	Topics to be covered	Reference Chap
L. 1	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. 2-3 P. 1	Matlab Programming	Variable Types; Built in functions; Plot tools; Writing functions; Control structures; Managing variables; Matrix operations;	T1: Ch. 1, 2, 3 and 4
L. 4-6	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	
P. 2	Matlab Programming	Matlab Programming	
L. 7-9	System of Linear Algebraic Equations	Direct Methods: Gauss Elimination Methods, LU Decomposition	T1: Ch.9
		Iterative Methods: Gauss-Seidel Method	T1: Ch.10/ R1 Ch. 3
P. 3		P2. Solution to Linear Algebraic Equations using Matlab	
L. 10-12	System of Ordinary difference Equations	ODE, Explicit Methods; R-K methods	T1. Ch. 25 & 26 /R1 Ch. 4
		Implicit method	
		Boundary Value problems	T1. Ch 27/ R1. Ch. 4
P. 4		P4. Solution to Sys. of ODEs using Matlab	
L. 13-15	System of Partial Differential Equation	Classification of PDE, boundary conditions, Developing PDE in Chemical Engg. Systems.	T1. PT. 8 & Ch. 29
		Numerical Differentiation:	T1. Ch. 23
		Control Volume Method. Initial & Boundary conditions	
P. 5		P.5. Solution to Sys. of PDEs using Matlab PDE Tool box	

L. 16-20	Linear System Analysis	State Space Models	T2. Ch. 9 R1. Sec. III
		Linearization of Non-linear Models	
		Solution of general state-space form, Eigen value & Eigen Vector	
		Solving linear n^{th} order ODEs	
		Introduction to Laplace transforms	
		Analysis of First & Higher order Systems	
P. 6 & 7		P. 6. Matlab Step function & Initial function.	
L. 21-30	Nonlinear System Analysis	Phase-Plane Analysis.	T1. Chap 10-12 R1. Sec. IV
		Introduction to Nonlinear dynamics	
		Bifurcation behavior for single	
P. 8-10		Matlab Simulink	
L. 31-40	Modeling and Simulation of Chemical Processes	Fluidized bed combustion modeling	Lichtner et al Surasani et al
		Reactive Transport in Porous Media	
		Introduction to Population Balance modeling	
		Granulation of API	
		Emulsification	
P. 8-14	CFD using ANSYS	Introduction to Work-Bench	R6. Ch, 9, 10 & 11 & ANSYS Manuals
		Geometry & Meshing techniques	
		Introduction to Fluent	
		Introduction to CFX	

L- Lecuture (1hr) **P- Practical (3hr)**

6. Evaluation Scheme:

EC No.	Evaluation Component	Duration	Weightage (%)	Date& Time	Nature of Component
1.	Test-I	1hr	15	8/9, 10.00--11 AM	100 % Closed
2.	Test-II	1hr	15	25/10, 10.00--11 AM	100 % Open
4.	Comprehensive	3hrs.	30	08/12 FN	Open + closed
5.	Practical Tests (P)		20	TBA	100% Open
6.	Project/Seminar/Viva		20	TBA	100% Open

7. Chamber Consultation Hour: To be announced in the class. Chamber: D204

8. Notices: All notices concerning this course will be displayed on the Chemical Engineering Notice Boards and CMS portal.

9. Make-up Policy: Make-up is granted only for genuine cases with valid justification and prior permission of Instructor-in-charge.

Instructor-in-Charge
Dr. Vikranth Kumar Surasani
CHE G 523