SEMESTER: S5

PROCESS MODELLING & SIMULATION

Course Code	PEPOT527	CIE Marks	40
Teaching Hours/Week (L: T:P: R)	3-0-0-0	ESE Marks	60
Credits	3	Exam Hours	2 Hrs. 30 Min.
Prerequisites (if any)	Basic Knowledge of Heat Transfer, Mass Transfer, And Fluid Flow Operations.	Course Type	Theory

Course Objectives:

1. To understand the important physical phenomena from the problem statement.
2. To develop model equations for the given system.
3. To apply suitable numerical simulation methods for the solution of models.

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SYLLABUS

Module No.	Syllabus Description	Contact Hours
1	**Introduction to Modelling and Fundamental Laws** Definitions of Modelling, Uses of Mathematical Modelling, Classification of Modelling Techniques-Basic Modelling Principles. Fundamental Laws of Chemical Engineering: -Energy Equations-Continuity Equation-Equation of Motion - Transport Equations -Equations of State Equilibrium States -Chemical Kinetics	9
2	**Reactor Modelling:** Models of Reactors-Mixing with Reaction-Reversible Reaction-Steam Jacketed Vessel-Isothermal Constant and Variable Holdup CSTR in Series	9
3	**Separation Process Modelling:** Models of Separation Processes: - Multicomponent Flash Drum-Ideal Binary Distillation Column - Multicomponent Distillation Column, Batch Distillation-Condensation	9

4	**Distributed System Modelling and Numerical Simulation Techniques:** Distributed System Modelling: Jacketed Tubular Reactor-Laminar Flow in a Pipe - Counter Current Liquid-Liquid Heat Exchanger Numerical Simulation Techniques: Finite Difference Method -Method of Weighted Residuals. Simulation of Gravity Flow Tank -CSTR in Series -Non-Isothermal CSTR	9

Course Assessment Method
(CIE: 40 marks, ESE: 60 marks)

Continuous Internal Evaluation Marks (CIE):

Attendance	Assignment/ Micro project	Internal Examination-1 (Written)	Internal Examination- 2 (Written)	Total
5	15	10	10	40

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End Semester Examination Marks (ESE)

In Part A, all questions need to be answered and in Part B, each student can choose any one full question out of two questions

Part A	Part B	Total
● 2 Questions from each module. ● Total of 8 Questions, each carrying 3 marks **(8x3 =24marks)**	● Each question carries 9 marks. ● Two questions will be given from each module, out of which 1 question should be answered. ● Each question can have a maximum of 3 sub divisions. **(4x9 = 36 marks)**	**60**

Course Outcomes (COs)

At the end of the course students should be able to:

Course Outcome		Bloom's Knowledge Level (KL)
CO1	Define the fundamental principles of mathematical modelling in chemical engineering.	**K1**
CO2	Develop and formulate mathematical models for various chemical processes, including reactors and separation processes.	**K3,K6**
CO3	Analyze and interpret the results obtained from model equations to understand the behaviour of chemical processes.	**K4**
CO4	Explain the numerical simulation techniques to solve complex process models and validate the results against theoretical and experimental data.	**K2**
CO5	Determine the Design and optimize chemical processes to improve efficiency and performance.	**K6**

Note*: K1- Remember, K2- Understand, K3- Apply, K4- Analyse, K5- Evaluate, K6- Create*

CO-PO Mapping Table:

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	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	1											
CO2	1	2		2								
CO3	2	2	1									
CO4	2											
CO5	1	2			3							

Text Books				
Sl. No	**Title of the Book**	**Name of the Author/s**	**Name of the Publisher**	**Edition and Year**
1	Chemical Process Modelling and Computer Simulation	Amiya K.Jana	Prentice Hall of India.	2008
2	Process Dynamics - Modelling Analysis and Simulation	Biquette W.B.	Prentice Hall of India.	1st Edition
3	Mathematical Modelling in Chemical Engineering,	Franks R.G. E	John Wiley.	1967
4	Chemical Engineering Dynamics - Modelling with PC Simulation	John Ingham et.al	VCH Publishers.	2nd Edition

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Reference Books				
Sl. No	**Title of the Book**	**Name of the Author/s**	**Name of the Publisher**	**Edition and Year**
1	Fundamentals and Modelling of Separation Processes	Holland C. D	Prentice Hall,	1975
2	Process Modelling Simulation and Control for Chemical Engineers	Luyben W. L	2nd Ed., McGraw Hill,	1990
3	Mathematical Modelling, Vol. 1: A Chemical Engineering Perspective (Process System Engineering),	Aris R	Academic Press,	1999
4	Process Modelling and Control in Chemical Engineering	Najim K	CRC,	1990

Video Links (NPTEL, SWAYAM…)	
Module No.	**Link ID**
1	Mathematical Modelling and Simulation of Chemical Engineering Processes by Prof. Sourav Mondal, IIT Kharagpur. This course covers mathematical modelling approaches, theoretical frameworks for heat, mass, and fluid flow, and includes simulation techniques (https://onlinecourses.nptel.ac.in/noc24_ch76/preview) (https://onlinecourses.nptel.ac.in/noc22_ch47/preview).
2	Chemical Process Control by Prof. S. Pushpavanam, IIT Madras. This course includes fundamental principles such as energy and continuity equations, equations of motion, transport equations, and equilibrium states
3	Chemical Reaction Engineering by Prof. Kannan Moudgalya, IIT Bombay. This course covers models of reactors, including mixing with reaction, reversible reactions, and steam jacketed vessels
4	Process Equipment Design by Prof. M. K. Jha, IIT Roorkee. This course includes models of separation processes like multicomponent flash drums and distillation columns

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