NIRMA UNIVERSITY

School of Engineering, Institute of Technology

B.Tech. in Chemical Engineering

Disciplinary Minor in Chemical Engineering

Third Year /Semester VI

Institute:	Institute of Technology
Name of Programme:	B. Tech. (Chemical Engineering)
Course Code:	3CH203DE24
Course Title:	Advanced Distillation Technologies
Course Type:	Elective-I
Year of introduction:	2024-25

L	T	Practical component			
		LPW	PW	W	S
3	-	2	-	-	-

Course Learning Outcomes (CLOs):

At the end of the course, the student will be able to –

1. analyse the process parameters related to distillation design and control (BL4)
2. make use of various technologies for the azeotropic distillation system (BL3)
3. develop the design of various advanced distillation technologies (BL3)
4. design and simulate advanced distillation columns (BL6)

Total Teaching hours: 45

Syllabus:

		Teaching hours
Unit I	**Basic Concepts in Distillation** Vapor–Liquid Equilibrium and VLE Non-ideality, Relative Volatility, Bubble Point Calculations, Analysis of Distillation Columns, Degrees of Freedom Analysis, McCabe-Thiele Method, Approximate Multicomponent Methods	**07**
Unit II	**Design, Control and Economics of Distillation** Design Principles, Operating Pressure, Heuristic Optimisation, Rigorous Optimisation, Energy Savings in Distillation Systems, Basics of Distillation Controls, Equipment Sizing and Costs, Utilities and Energy Costs, Cost of Chemicals.	**08**
Unit III	**Homogeneous Azeotropic Distillation** Azeotropes and its Importance in Distillation Design, Ternary Diagrams, Residue Curve Maps for Multicomponent Mixtures, Feasibility, Product Distribution and Sequences, Conceptual Design Method, Extractive Distillation Basics, Basics of Pressure Swing Distillation, Salt Distillations, Case Studies.	**14**
Unit IV	**Heterogeneous Azeotropic Distillation** Introduction, Phase Diagrams, Residue Curve Maps, Distillation System Synthesis, Other Classes of Entrainers.	**08**
Unit V	**Basics of Advanced Distillation Technologies**	**08**

Principle and Design Concepts, Applications of Advanced Distillation Technologies like Dividing Wall Column, Reactive Distillation, Cyclic Distillations, Heat Integrated Distillation Columns, etc., Case Studies, Introduction to Batch Distillation Design and Simulations.

Self Study:

The self study contents will be declared at the commencement of semester. Around 10% of the questions will be asked from self study contents.

Laboratory Work:

Laboratory work will be based on the above content of course.

Suggested Readings/References:

1. Kiss A. A., Advanced Distillation Technologies, Design Control and Applications, John Willey and Sons Ltd., Publications.
2. Doherty M. F., Malone M. F., Fair, Conceptual Design of Distillation Systems, McGraw Hill Publications.
3. Luyben W.L., Distillation Design and Control using Aspen Simulation, Willey Publications.
4. Douglas J. M., Conceptual Design of Chemical Processes, McGraw Hill Publications.

L= Lecture, T=Tutorial, P= Practical, C=Credit

List of Experiments:

Sr. No.	Practical	No. of Hours
1	To predict VLE for any given binary system using a process simulator	2
2	Regressing VLE data to obtain binary interaction parameters for thermodynamic models	4
3	Simulating binary and multi-component distillation systems	4
4	Analysing the effect of binary interaction parameter on simulation of distillation column	2
5	To generate Residue Curve Maps for a given system	2
6	Simulating Azeotropic System	4
7	Simulating Extractive Distillation System	4
8	Costing Analysis of Conventional Distillation System	4

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Disciplinary Minor B.Tech. in Chemical Engineering
Third Year /Semester VI

Institute:	Institute of Technology
Name of Programme:	B. Tech. Chemical Engineering
Course Code:	3CH503DE24
Course Title:	Computational Fluid Dynamics
Course Type:	Elective
Year of introduction:	2023-2024

L	T	Practical component			
		LPW	**PW**	**W**	**S**
3	1	0	-	-	-

Course Learning Outcomes (CLOs):

At the end of the course, the students will be able to –

1. examine aerodynamic flow solutions and compare existing CFD software (BL4)
2. analyse the flow problem, use a CAD programme to model solidly, and use a meshing tool to create grids. (BL4)
3. apply Navier-Stokes equations and use finite difference method (BL3)
4. apply CFD software to engineering flow problems. (BL3)

Syllabus: **Total Teaching hours:45**

Unit I **Fundamental and Basic Concept of CFD**

Illustration of CFD approach, future, Governing equations (GE's) of Fluid dynamics: Modeling of flow, control volume concept, substantial derivative, physical meaning of the divergence of velocity. Continuity equation, momentum equation, energy equation and its conservation form. Equations for viscous flow (Navier-Stokes equations), equations for inviscid flow (Euler equation). Different forms of GE's, initial and boundary conditions.

Unit II **Discretisation**

FVM for 1D steady state diffusion, 2D steady state diffusion, 3d steady state diffusion. Solution of discretised equations - TDMA scheme for 2D and 3D flows. FVM for 1D steady state convection-diffusion, Central differencing scheme, Conservativeness, Boundedness, Transportiveness, upward differencing scheme, Hybrid differencing scheme for 2D and 3D convection-diffusion, Power-law scheme, QUICK scheme.

Unit III **Solution Methods**

Discretisation schemes for pressure, momentum, and energy equations – Explicit and implicit Schemes, Solution methods of discretised equations - Tridiagonal matrix algorithm (TDMA) Application of TDMA for 2D problems potential flow - Stream and vorticity function. Unsteady flows - Crank Nicholson scheme, solution of Navier-Stokes equations. 8

Unit IV CFD Solution Procedure

Problem setup-creation of geometry, mesh generation, selection of physics and fluid properties, initialisation, solution control and convergence monitoring, results reports and visualisation. Case Studies: Benchmarking, validation, Simulation of CFD problems by use of general CFD software, Simulation of coupled heat, mass and momentum transfer problem. 8

Self-Study:

Self-study contents will be declared at the commencement of the semester. Around 10 % of the questions will be asked from the self-study contents.

Tutorial Work:

Tutorial work will be based on the above content of course.

Suggested Readings/ References:

1. P.S. Ghosdastidar, Computer Simulation of Flow and Heat Transfer, Tata McGraw-Hill.
2. Muralidhar, K., and Sundararajan, T. Computational Fluid Flow and Heat Transfer, Narosa Publishing House.
3. Niyogi, P. Chakrabarty, S.K. and Laha, M.K., Introduction to computational fluid dynamics,
   Pearson education.
4. Suhas V. Patankar, Numerical Heat Transfer and Fluid Flow, Taylor and Francis
5. S.K. Gupta, Numerical Methods for Engineers, New Age Publishers.

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Third Year /Semester VI

Institute:	Institute of Technology
Name of Programme:	B. Tech. (Chemical Engineering)
Course Code:	3CH605IE24
Course Title:	Computational Tools in Process Engineering
Course Type:	Elective
Year of introduction:	2024-25

L	**T**	**Practical component**			
		LPW	**PW**	**W**	**S**
2	1	2	-	-	-

Course Learning Outcomes (CLOs):

At the end of the course, students will be able to-

1. make use of modeling basics for process engineering (BL3)
2. analyse the use of various simulation software in process engineering (BL4)
3. compute various properties theoretically and using computational tools (BL3)
4. analyze simulations of basic unit operations and optimisation problems (BL4)

Syllabus:		**Teaching Hours**
Unit I	**Basics of Process Modelling and Simulations** General Aspects of Modelling and Simulation, Process Synthesis and Process Analysis, Study and Applications of Fundamental Laws, Introduction to Regression Analysis.	**05**
Unit II	**Introduction to Various Software/Simulators** Introduction to software like MATLAB, POLYMATH etc., Introduction to Process Simulators and Their usage in Process Engineering. Approaches to Process Simulations, Basics of Sequential Modular Approach, Introduction to Partitioning and Tearing.	**08**
Unit III	**Computing Various Properties using Computational Tools** Codes for Estimation of Various Physical Properties, Solution of Problems Based on Thermodynamics, Solution of Equation of State and Activity Coefficient Models, and Problems Based on Basic Flow and Pressure Losses in Pipelines and Fittings.	**04**
Unit IV	**Distillation and Reactor Simulations using Process Simulators** Basic Theory of Distillation Design, Simulations of Distillation Columns, Different Kinds of Reactors in Simulations, Case Study Problems for Simulations of Reactors.	**08**
Unit V	**Process Optimisation** Various Optimisation Techniques, Applications in Chemical Engineering, Solutions to Problems using Different Computational Tools.	**05**

Self Study:
The self study contents will be declared at the commencement of semester. Around 10% of the questions will be asked from self study contents.

Laboratory Work:
Laboratory work will be based on the above content of course.

Tutorial Work:
Tutorial work will be based on the above content of course.

Suggested Readings/References:

1. Biegler L. T., Grossman I. E., Westerberg A. W., Systematic Methods of Chemical Process Design, Prentice Hall Publication.
2. Ramirez W. F., Computational Methods for Process Simulation, Butterworth-Heinemann
3. Martin M M, Introduction to Software for Chemical Engineers, CRC Press.

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List of Experiments:

Sr. No.	Practical	No. of Hours
1	To familiarise students with basic inputs required for MATLAB	2
2	Write simple codes for solving chemical engineering models using MATLAB	4
3	Solve ordinary differential equations with the help of MATLAB	2
4	To familiarise students with basic inputs required for steady-state simulations using CHEMCAD	2
5	Perform steady-state simulations of various basic unit operations part I	2
6	Perform steady-state simulations of basic unit operations- part II	4
7	Make students learn how to simulate simple reactors in a process simulator	4
8	To familiarise students with various logical operators of a process simulator	4
9	Perform process simulations of a binary distillation column	2
10	Perform Optimisation of chemical engineering problems	2