CURRICULUM & SYLLABI

M.Tech. CHEMICAL ENGINEERING

Effective from AY: 2024-25



NATIONAL INSTITUTE OF TECHNOLOGY WARANGAL

WARANGAL, TELANGANA

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Vision and Mission of the Institute
National Institute of Technology Warangal

VISION

Towards a Global Knowledge Hub, striving continuously in pursuit of excellence in Education, Research, Entrepreneurship and Technological services to the society

MISSION

- Imparting total quality education to develop innovative, entrepreneurial and ethical future professionals fit for globally competitive environment.
- Allowing stake holders to share our reservoir of experience in education and knowledge for mutual enrichment in the field of technical education.
- Fostering product-oriented research for establishing a self-sustaining and wealth creating centre to serve the societal needs.

Vision and Mission of the Department
Chemical Engineering

VISION

To attain global recognition in research and training students for meeting the challenging needs of chemical & allied industries and society.

MISSION

- Providing high quality undergraduate and graduate education in tune with changing needs of industry.
- Generating knowledge and developing technology through quality research in frontier areas of chemical and interdisciplinary fields.
- Fostering industry-academia relationship for mutual benefit and growth.

Program: M.Tech. Chemical Engineering

Program Educational Objectives

PEO-1	Pursue successful industrial, academic and research careers in specialized fields of Chemical Engineering.
PEO-2	Apply the knowledge of advanced topics in Chemical Engineering to meet contemporary needs of industry and research.
PEO-3	Use modern software tools for design of processes and equipment.
PEO-4	Identify issues related to ethics, society, safety, energy and environment in the context of Chemical Engineering applications.
PEO-5	Engage in ongoing learning and professional development through pursuance of higher education and self-study.

Program Articulation Matrix

PEO / Mission Statements	PEO-1	PEO-2	PEO-3	PEO-4	PEO-5
Providing high quality education in tune with changing needs of industry.	3	3	3	2	-
Generating knowledge and developing technology through quality research in frontier areas of chemical and interdisciplinary fields.	3	2	2	1	-
Fostering industry-academia relationship for mutual benefit and growth.	3	2	2	-	2

1 - Slightly; 2 - Moderately; 3 - Substantially

Program: M.Tech. Chemical Engineering

Program Outcomes

PO-1	Independently carry out research /investigation and development work to solve practical problems.
PO-2	Write and present a substantial technical report/document.
PO-3	Model chemical engineering processes including multi-component mass transfer, multi-phase momentum transfer and multi-mode heat transfer from advanced engineering perspective.
PO-4	Apply modern experimental, computational and simulation tools to minimize the cost & energy by taking care of environment health and safety in Chemical and allied engineering industries.
PO-5	Contribute effectively in a team and demonstrate leadership skills with professional ethics.
PO-6	Pursue life-long learning, updating knowledge and skills for professional and societal development.

CURRICULUM
M.Tech. Chemical Engineering

1st Semester

S.No.	Code	Course Title	L-T-P	Credits
1	CH16001	Advanced Transport Phenomena	3-0-0	3
2	CH16003	Advanced Reaction Engineering	3-0-0	3
3	CH16005	Data Analytics and Machine Learning	3-0-0	3
4		Professional Elective - I	3-0-0	3
5		Professional Elective - II	3-0-0	3
6	CH16007	Data Analytics and Machine Learning Laboratory	0-1-2	2
7	CH16009	Material Synthesis and Applications Laboratory	0-1-2	2
			Total Credits	19

2nd Semester

S.No.	Code	Course Title	L-T-P	Credits
1	CH16002	Computational Fluid Dynamics	3-0-0	3
2	CH16004	Steady State Process Simulation	3-0-0	3
3		Professional Elective – III	3-0-0	3
4		Professional Elective - IV	3-0-0	3
5		Professional Elective - V	3-0-0	3
6	CH16006	Process Synthesis and Simulation Laboratory	0-1-2	2
7	CH16008	Flow Modelling and Simulation Laboratory	0-1-2	2
8	CH16096	Minor Project	0-0-0	2
			Total Credits	21

3rd Semester

S.No.	Code	Course Title	L-T-P	Credits
1	CH17089	Seminar and Technical Writing	0-0-0	2
2	CH17091	Summer Internship / Research Experience	0-0-0	2
3	CH17093	Comprehensive Viva-voce	0-0-0	2
4	CH17097	Dissertation: Part A	0-0-0	8
			Total Credits	14

4th Semester

S.No.	Code	Course Title	L-T-P	Credits
1	CH17098	Dissertation: Part B	0-0-0	12
			Total Credits	12

Professional Elective Courses:

Professional Electives – I & II		
S.No.	**Code**	**Course Title**
1	CH16021	Circular Economy for Sustainable Development
2	CH16023	Advanced Mass Transfer
3	CH16025	Computational Techniques
4	CH16027	Advanced Process Modelling
5	CH16029	Chemical Process Synthesis
6	CH16031	Safety Analysis in Process Industries
7	CH16033	Green and Cleaner Technologies
8	CH16035	Industrial Instrumentation
9	CH16037	Solid Waste Management
10	CH26001	Sustainable Energy Engineering
11	CH26003	Hydrogen Generation and Storage
12	CH26021	Fuel Cell Systems
13	CH26027	Waste to Energy

Professional Electives – III, IV & V		
S.No.	**Code**	**Course Title**
1	CH16022	Wastewater Treatment
2	CH16024	Engineering Optimization
3	CH16026	CO_2 Capture, Sequestration and Utilization
4	CH16028	Energy Audit and Conservation
5	CH16030	Novel Separation Techniques
6	CH16032	Characterization Techniques
7	CH16034	Modelling and Simulation of Wastewater Treatment Processes
8	CH16036	Process Intensification
9	CH16038	Electrochemical Engineering
10	CH16040	Advanced Physicochemical Treatment Technologies
11	CH16042	Molecular Thermodynamics

12	CH16044	Statistical Design of Experiments
13	CH16046	Thermoset Polymer Composites
14	CH16048	Molecular Simulations
15	CH16050	Heat Integration and Process Scheduling
16	CH16052	Statistical Thermodynamics
17	CH16054	Computational Catalysis
18	CH16060	Advanced Process Control
19	ME16062	Thermal Energy Storage
20	CH26002	Electrochemical Energy Storage Systems

SYLLABI

M.Tech. Chemical Engineering

1st Semester

CH16001 **3-0-0 (3)**

Advanced Transport Phenomena

Pre-Requisites: **None**

Course Outcomes:

CO-1	Perform momentum, energy and mass balances for a given system at macroscopic and microscopic scale
CO-2	Solve the governing equations to obtain velocity, temperature and concentration profiles
CO-3	Model the momentum, heat and mass transport under turbulent conditions
CO-4	Develop analogies among momentum, energy and mass transport

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	1	3	3	-	2
CO-2	3	1	3	3	-	3
CO-3	3	1	3	3	-	3
CO-4	3	1	3	3	-	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Equations of Change for Isothermal Systems: Equation of Continuity, Equation of Motion, Equation of Mechanical Energy, Equations of Change in terms of the Substantial Derivative, Use of the Equations to solve Flow Problems, Dimensional Analysis of the Equations of Change.

Velocity Distributions with more than one Independent Variable: Time Dependent Flow of Newtonian Fluids. Velocity Distributions in Turbulent Flow-Comparisons of Laminar and Turbulent Flows, Time Smoothed Equations of Change for Incompressible Fluids, Time Smoothed Velocity Profile near a wall, Empirical Expressions for the Turbulent Momentum Flux, Turbulent Flow in Ducts.

Macroscopic Balances for Isothermal Systems: The Macroscopic Mass Balance, The Macroscopic Momentum Balance, The Macroscopic Mechanical Energy Balance, Estimation of the Viscous loss, Use of the Macroscopic Balances for Steady-State Problems, Derivation of the Macroscopic Mechanical Energy Balance.

Equations of Change for Non-Isothermal Systems: The Energy Equation, Special forms of the Energy Equation, The Boussinesq Equation of Motion for Forced and Free Convection, Useof the Equations of change to Solve Steady-State Problems, Dimensional Analysis of the Equations of Change for Non-Isothermal Systems.

Temperature Distributions in Solids and in Laminar Flow: Heat Conduction with an Electrical Heat Source, Heat Conduction with a Viscous Heat Source. Temperature Distributions with more than One Independent Variable - Unsteady Heat Conduction in Solids,Temperature Distributions in Turbulent Flow - Time-Smoothed Equations of Change for Incompressible Non-Isothermal Flow, Time-Smoothed Temperature Profile near a Wall, Empirical Expressions for the Turbulent Heat Flux Temperature Distribution for Turbulent Flow in Tubes.

Macroscopic Balances for Non-Isothermal Systems: Macroscopic Energy Balance, Macroscopic Mechanical Energy Balance, Use of the Macroscopic Balances to Solve SteadyState Problems with Flat Velocity Profiles.

Concentration Distributions in Solids and in Laminar Flow: Shell Mass Balances Boundary Conditions, Diffusion through a Stagnant Gas Film, Diffusion with a Heterogeneous Chemical Reaction. Concentration Distributions with more than One Independent Variable: Time-Dependent Diffusion. Concentration Distributions in Turbulent Flow - Concentration Fluctuations and the Time-Smoothed Concentration, Time-Smoothing of the Equation of Continuity, Semi-Empirical Expressions for the Turbulent Mass Flux.

Interphase Transport in Multi-Component Systems: Definition of Transfer Coefficients in One Phase, Analytical Expressions for Mass Transfer Coefficients, Correlation of Binary Transfer Coefficients in One Phase, Definition of Transfer Coefficients in Two Phases, Mass Transfer and Chemical Reactions.

Macroscopic Balances for Multi-Component Systems: Macroscopic Mass Balances, Macroscopic Momentum, Use of the Macroscopic Balances to solve Steady-State Problems.

Learning Resources:

Text Books:

1. Bird R. B., Stewart W. E. and Light Foot E. N., Transport Phenomena, John Wiley & Sons,2007, 2nd Edition.
2. Geankopolis C. J., Transport Processes and Unit Operations, Prentice Hall (India) Pvt. Ltd., 2004, 4th Edition.
3. Mauri Robert., Transport Phenomena in Multiphase Flows, Springer InternationalPublishing, 2015.

Reference Books:

1. Koichi Asano, Mass Transfer: From Fundamentals to Modern Industrial Applications, Wiley-VCH, 2006.
2. Thomson W. J., Transport Phenomena, Pearson education, 2001.
3. W.M. Deen, Analysis of Transport Phenomena, Oxford University Press, 2013, 2nd Edition.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103106068
2. https://ocw.tudelft.nl/courses/advanced-transport-phenomena/?view=lectures&paging=1

CH16003 **3-0-0 (3)**

Advanced Reaction Engineering

Pre-Requisites: **None**

Course Outcomes:

CO-1	Evaluate heterogeneous reactor performance considering mass transfer
CO-2	Determine the concentration profiles in multiphase reactors
CO-3	Estimate the performance of multiphase reactors under non-isothermal conditions
CO-4	Evaluate the role of modern reactor technologies for mitigation of global warming

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	-	-	2	1	3	-
CO-2	-	-	2	1	3	-
CO-3	-	-	2	1	3	-
CO-4	-	-	2	1	3	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Non-Isothermal reaction modelling in CSTR & Batch, Semi-Batch reactor: Energy Balance equations for CSTR, PFR and Batch reactors. Unsteady state non-isothermal reactor design, adiabatic operation in batch, Heat effects in semi-batch. Auto thermal reactors.

Catalyst preparation and characterization: Catalysis - Nature of catalysis, methods of evaluation of catalysis, factors affecting the choice of catalysts, promoters, inhibitors, and supports, catalyst specifications, preparation and characterization of catalysts, surface area measurement by BET method, pore size distribution, catalyst, poison, mechanism and kinetics of catalyst, deactivation.

Heterogeneous Reactors: Catalytic wall reactor, monolithic reactors, limiting steps: reactions and mass transfer limiting, Porous catalyst on tube wall reactors, Design of packed bed porous catalytic reactors: Mass transfer limited reactions in Packed bed, Transport and Reactions, Gradients in the reactors: temperature. Fluidized bed reactor modelling: Class III Modelling the Bubbling Fluidized Bed Reactor (BFB), The Kunii-Levenspiel bubbling bed model,Gas Flow Around and Within a Rising Gas Bubble in a Fine particle BFB, Reactor performance of BFB. CVD, trickle bed reactors. Polymerization techniques and reactors.

Application of Population Balance Equations for reactor modelling: Particle size distribution, Distribution Functions in Particle Measuring Techniques, Particle distribution model in colloidal particle synthesis in batch reactor, Moments of Distribution, Nucleation rate based on volumetric holdup versus crystal growth rate.

Reaction engineering and mitigation of Global warming: CO_2 absorption, different techniques of mitigation of CO_2, Recent advancements, automotive monolith catalytic converter example, removal and utilization of CO_2 for thermal power plants.

Learning Resources:

Text Books:

1. Fogler H.S., Elements of Chemical Reaction Engineering, Prentice Hall of India, 2008.

2. Levenspiel O., Chemical Reaction Engineering, John Wiley & Sons, 1999, 3rd Edition.
3. Fromment G.F., Bischoff K.B, Chemical Reactor Analysis and Design, John Wiley, 2010.

Reference Books:

1. Schmidt L.D., The Engineering of Chemical Reactions, Oxford, 2007.
2. Harriott P., Chemical Reactor Design, CRC Press, 2002.
3. James J. Carberry, Chemical and catalytic reaction engineering, Dover Publications, 2001.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103101001

CH16005 **3-0-0 (3)**

Data Analytics and Machine learning

Pre-Requisites: **None**

Course Outcomes:

CO-1	Demonstrate proficiency with statistical analysis of data
CO-2	Use inferential statistics for decision making
CO-3	Apply supervised learning for classification and regression problems
CO-4	Apply unsupervised learning for clustering

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	3	1	2	1	2
CO-2	3	-	1	2	1	2
CO-3	3	-	1	2	1	2
CO-4	3	-	1	2	1	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Data Quality and Pre-processing: Distance measures, dimensionality reduction, principal component analysis (PCA).

Descriptive Statistics: Graphical approach - Frequency tables, relative frequency tables, grouped data, pie chart, barchart, histograms, ogives, stem and leaf plots, box plots, dot diagram, scatter plots, Pareto diagram.

Measure of Central Tendency and Dispersion - Arithmetic mean, median and mode, variance, standard deviation, quartiles, range, mean absolute deviation, coefficient of variation, Z scores,normal distribution, confidence interval estimation.

Probability Distribution and Inferential Statistics: Random variables, probability distributions, hypothesis testing, single sample test, two sample test, Type I error, Type II error, Analysis of Variance (ANOVA).

Supervised learning: Linear regression, ridge regression, Lasso regression, logistic regression, multiple linear regression, goodness of fit, bias–variance trade off, k-nearest neighbors' algorithm, linear discriminant analysis, classification and regression trees and pruning, support vector machines, random forest, Naive Bayes, Introduction to Neural networks and deep learning.

Unsupervised learning: Cluster analysis – K Means, hierarchical, DBSCAN.

Time series analysis: Auto-Regressive (AR), Moving Average (MA), Auto Regressive Moving Average (ARMA), Auto-Regressive Integrated Moving Average (ARIMA).

Practical applications to different engineering systems.

Learning Resources:

Text Books:

1. Douglas C. Montgomery, George C. Runger, Applied Statistics and Probability for Engineers, John Wiley & Sons Inc., 2016, 6th Edition.
2. Trevor Hastie, Robert Tibshirani, Jerome Friedman, The Elements of Statistical Learning, Springer, 2009, 2nd Edition.
3. Ethem Alpaydın, Introduction to Machine Learning, MIT Press, 2014, 3rd Edition.

Reference Books:

1. João Mendes Moreira, André C. P. L. F. deCarvalho, Tomáš Horváth, A General Introduction to Data Analytics, Wiley, 2019.
2. Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, Vipin Kumar, Introduction to Data Mining, Pearson, 2019, 2nd Edition.

Other Suggested Readings:

1. https://nptel.ac.in/courses/106107220
2. https://nptel.ac.in/courses/110106072

CH16007 **0-1-2 (2)**

Data Analytics and Machine learning Laboratory

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the python programming, data handling and standard library functions
CO-2	Find different properties of given data by central tendency, dispersion and inferential statistics
CO-3	Solve supervised and unsupervised machine learning problems
CO-4	Forecast and interpret the time series data

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	2	-	2	-	1
CO-2	3	2	-	2	-	1
CO-3	3	2	-	2	-	1
CO-4	3	2	-	2	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

1. Introduction to Python: Basics of software handling, variables, functions, libraries (numpy, pandas)
2. Introduction to Python: loops, data structures, file handling
3. Data preprocessing and data cleaning
4. Descriptive statistics
5. Principle component analysis (PCA)
6. Random variables and probability distributions
7. Hypothesis testing
8. Supervised learning: Regression (liner, polynomial, multiple, Lasso, Ridge)
9. Supervised learning: Support vector machines (SVM) and K-nearest neighbor (KNN)
10. Supervised learning: Random forest (RF), other new methods
11. Unsupervised learning: K-means clustering, hierarchical clustering
12. Unsupervised learning: DBSCAN
13. Time series analysis

Learning Resources:

Reference Books:

1. McKinney W., Python for Data Analysis, O'Reilly Media, 2022, 3rd Edition.
2. Sebastian R., Python Machine Learning, 2017, 2nd Edition.
3. Huang C., Petukhina, A., Applied Time Series Analysis and Forecasting with Python (Statistics and Computing), 2022, 1st Edition.

CH16009 **0-1-2 (2)**

Materials Synthesis and Applications Laboratory

Pre-Requisites: **None**

Course Outcomes:

CO-1	Develop the ability to accurately perform conductometric, potentiometric titrations
CO-2	Conduct cyclic voltammetry and electrodeposition experiments and analyze oxidation, reduction, and corrosion processes
CO-3	Synthesize carbon xerogels and thin films
CO-4	Analyze the concentration of substance using spectroscopy technique

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	3	1	1	1	3
CO-2	3	3	1	1	1	3
CO-3	3	3	1	1	1	3
CO-4	3	3	1	1	1	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

1. Conductometric Titration for Concentration Determination
2. Potentiometric Titration for Concentration Determination
3. Electrodeposition
4. Cyclic Voltammetry to Determine Oxidation and Reduction Reaction Potential
5. Electrochemical Measurement of Corrosion Rate
6. Structural Color and Wettability using Soft-lithography Technique
7. Synthesis of Activated Carbon from Coconut Shell
8. Thin Film Preparation using Spin and Dip Coating Techniques
9. Synthesis of Resorcinol-Formaldehyde Xerogel
10. Spectroscopic Determination of Methylene Blue Dye Concentration

Learning Resources:

Reference Books:

1. Lab manuals.

2nd Semester

CH16002 **3-0-0 (3)**

Computational Fluid Dynamics

Pre-Requisites: **None**

Course Outcomes:

CO-1	Develop governing equations of fluid flow and heat transfer
CO-2	Discretize the equations using finite difference and finite volume formulation
CO-3	Solve the discretized equations
CO-4	Implement pressure velocity coupling algorithms
CO-5	Generate grid for a given geometry

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	3	2	1	1
CO-2	2	1	3	3	1	1
CO-3	2	1	3	3	1	1
CO-4	2	1	3	3	1	1
CO-5	2	1	3	3	1	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: CFD approach, Need for CFD.

Governing equations of fluid flow and heat transfer: Introduction to Laws of conservation: Mass, Momentum, Energy equations; Initial and boundary conditions; Conservative form – Differential and Integral forms of general transport equations; Application of Navier-Stokes equations; Classification of physical behaviors – Classification of fluid flow equations.

Discretization of equations: Finite difference / volume methods – 1D, 2D and 3D Diffusion problems, Convection and diffusion problems; Properties of discretization schemes- Central, upwind, hybrid and higher order differencing schemes.

Solution methods of discretized equations: Tridiagonal matrix algorithm (TDMA); Application of TDMA for 2D and 3D problems; Iterative methods.

Pressure velocity coupling algorithms in steady flows: Staggered grid; SIMPLE, SIMPLEC and PISO.

Unsteady flows: Explicit scheme, Crank Nicholson scheme, fully implicit scheme, Pressure-velocity coupling algorithms in unsteady flows.

Turbulence modelling: Prandtl mixing length mode - One equation model, k - ε model.

Grid generation: Structured and unstructured grids, Grid generation methods.

Learning Resources:

Text Books:

1. H.K. Versteeg, W. Malalasekera, An Introduction to Computational Fluid Dynamics – The Finite Volume Method, Prentice Hall, 2007, 2nd Edition.
2. John D. Anderson, Jr., Computational Fluid Dynamics – The Basics with Applications, McGraw Hill Education, 2017.

Reference Books:

1. C. Hirsch, Numerical Computation of Internal and External Flows: The Fundamentals of Computational Fluid Dynamics: 1, Wiley, 2007, 2nd Edition.
2. J.H. Ferziger, M. Peric, R.L. Street, Computational Methods for Fluid Dynamics, Springer, 2019, 4th Edition.
3. Sreenivas Jayanti, Computational Fluid Dynamics for Engineers and Scientists, Springer, 2018, 1st Edition.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103106119
2. https://www.cfd-online.com

CH16004 **3-0-0 (3)**

Steady State Process Simulation

Pre-Requisites: **None**

Course Outcomes:

CO-1	Analyze the role and importance of property estimation methods in process simulation
CO-2	Determine the degrees of freedom for a given stream, process unit and flowsheet
CO-3	Apply suitable mathematical methods for solving sparse sets of equations, partitioning & precedence ordering and tear stream sets
CO-4	Carry out steady state process simulation using sequential modular approach and equation-oriented approach
CO-5	Apply convergence promotion techniques for both sequential and simultaneous convergence loops

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	-	3	3	1	1
CO-2	2	-	2	3	-	1
CO-3	3	-	3	3	-	1
CO-4	3	-	2	3	-	1
CO-5	3	-	2	3	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Steady-state flowsheeting and the design process, the total design project.

Flowsheeting on the computer: Motivation for development, Developing a simulation model, Approaches to flowsheeting systems-examples.

Solving linear and nonlinear algebraic equations: Solving one equation in one unknown, Solution methods for linear equations, General approaches to solving sets of nonlinearequations, Solving sets of sparse nonlinear equations.

Physical property service facilities: The data cycle, Computerized physical property systems, Physical property calculations.

Degrees of freedom in a flowsheet: Degrees of freedom, Independent stream variables, Degrees of freedom for a stream and a unit, Degrees of freedom for a flowsheet.

The sequential modular approach to flowsheeting: The solution of an example flowsheeting problem, Other features: Handling design specifications, information streams and control blocks.

Convergence of tear streams: Sequential convergence and simultaneous convergence, Partitioning and precedence ordering set of equations and a flowsheet, tearing a flowsheet, Finding the best tear set family or tear set with minimum number of tears.

Flowsheeting by equation solving methods based on tearing: An example system based on equation solving, A complex example of selecting decision and tear variables for a flowsheet, Handling the iterated variables.

Simulation by linear methods: Introduction to linear simulation, Application to staged operations, Application to management problem.

Learning Resources:

Text Books:

1. Westerberg A. W., Hutchison H. P., Motard R. L., Winter P., Process Flowsheeting, Cambridge University Press, 2011.

Reference Books:

1. Ivan Dano Gill Chaves, Javier Ricardo Guevara Lopez, Jpose Luis Garcia Zapata, Alexander Leguizamon Robayo, Gerardo Rodrigue Nino, Process Analysis and Simulation in Chemical Engineering, Springer, 2016.
2. Babu B. V., Process Plant Simulation, Oxford University Press, 2004.
3. Mariano Martin Martin, Introduction to Software for Chemical Engineers, CRC Press, 2015.

CH16006 **0-1-2 (2)**

Process Synthesis and Simulation Laboratory

Pre-Requisites: **None**

Course Outcomes:

CO-1	Estimate thermodynamic properties
CO-2	Simulate Mixer, splitter, heat exchanger, pump, compressor, flash unit, reactors, distillation columns, calculator block and solid handling units
CO-3	Apply sensitivity, design specification and case study tools
CO-4	Optimize process flowsheets using sequential modular approach as well as equation-oriented approach
CO-5	Perform dynamic simulation, pinch analysis and cost estimation

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	2	3	3	1	1
CO-2	3	2	3	3	1	1
CO-3	3	2	3	3	1	1
CO-4	3	2	3	3	1	1
CO-5	3	2	3	3	1	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Solve the following steady state simulation exercises:

1. Physical property estimations
2. Simulation of individual units like, mixers, splitters, heat exchangers, flash columns and Reactors
3. Design and rating of heat exchangers
4. Design and rating of distillation columns
5. Mass and Energy balances
6. Sensitivity and design Spec tools
7. Simulation of a flowsheet
8. Simulation exercises using calculator block
9. Process optimization
10. Simulation using equation-oriented approach
11. Simulation of processes involving solids
12. Pinch analysis
13. Dynamic simulation
14. Cost estimation

Learning Resources:

Reference Books:

1. Lab manuals / Exercise sheets.
2. A. K. Jana, Chemical Process Modelling and Computer Simulation, Prentice Hall India, 2018, 3rd Edition.
3. Thomas A. Adams II, Learn Aspen Plus in 24 Hours, McGraw Hill Education, 2018.
4. Juma Haydary, Chemical Process Design and Simulation - Aspen Plus and Aspen HYSYS Applications, Wiley, 2019.

CH16008 **0-1-2 (2)**

Flow Modelling and Simulation Laboratory

Pre-Requisites: **None**

Course Outcomes:

CO-1	Solve heat/mass/momentum balance equations using ANSYS CFD / COMSOL Multiphysics Software
CO-2	Visualize velocity/temperature/concentration distribution
CO-3	Analyse flow/heat/mass transfer in pipelines /process equipment
CO-4	Carry out sensitivity study for a flow process

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	2	3	3	2	2
CO-2	1	2	3	3	2	2
CO-3	1	2	3	3	2	2
CO-4	1	2	3	3	2	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

1. Step-by-step demonstration of CFD approach using Excel / MATLAB coding
2. Simulation using ANSYS CFD / COMSOL
   - i. Laminar flow through a pipe
   - ii. Turbulent flow through a pipe
   - iii. Flow past a cylinder/sphere
   - iv. Lid-driven cavity flow
   - v. Natural convection between vertical walls
   - vi. Double pipe heat exchanger
   - vii. Flow through Packed bed
   - viii. RTD determination in tubular reactor
   - ix. Conversion in PFR/Tubular reactor
   - x. Fluidization
   - xi. Reaction & Diffusion in and around a catalyst particle
   - xii. Effective thermal diffusivity/conductivity of granular material
   - xiii. Rayleigh Bernard Convection
   - xiv. Flow through micro-channels with obstacles like air bubbles

Out of all experiments, 8-10 experiments are offered.

Learning Resources:

Reference Books:

1. Exercise sheets / Lab manuals.
2. Ansys fluent user's guide.
3. COMSOL multiphysics documentation.

Other Suggested Readings:

1. https://www.cfd-online.com/Forums/

CH16096 **0-0-0 (2)**

Minor Project

Pre-Requisites: **None**

Course Outcomes:

CO-1	Apply engineering principles to real-world projects
CO-2	Plan and monitor project tasks individually or as a team
CO-3	Demonstrate practical experience in project execution
CO-4	Communicate project findings clearly through reports and presentations

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	-	3	3	2	2
CO-2	2	-	-	-	3	-
CO-3	3	-	2	2	-	3
CO-4	1	3	-	-	3	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Description:

Students are expected to choose real world or relevant problems and apply the engineering principles learned, to solve the problem through building prototypes or simulations or writing codes or establishing processes/synthesis/correlations etc.

Evaluation Criteria:

The student will be evaluated by the panel based on the below criteria.

Criteria	Description	Weightages
I	Identification of Problem Domain	20 marks
II	Study of Existing Systems and establishing clear objectives	20 marks
III	Planning of project and work distribution within the team	10 marks
IV	Proper Documentation and Technical Writing	20 marks
V	Presentation and Response to questions	30 marks

Evaluation Criteria-CO Mapping

CO / Criteria	CO-1	CO-2	CO-3	CO-4
I	X			
II	X			
III		X	X	
IV				X
V				X

3rd Semester

CH17089 **0-0-0 (2)**

Seminar and Technical Writing

Pre-Requisites: **None**

Course Outcomes:

CO-1	Consolidate ideas based on expert talks attended
CO-2	Prepare a well-organized report employing elements of critical thinking and technical writing
CO-3	Demonstrate the ability to describe, interpret and analyze the subject matter and develop competence in presenting

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	-	2	-	-	-	-
CO-2	2	3	-	-	3	2
CO-3	2	3	-	-	3	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Description:

In Seminar and Technical Writing, every student is expected to prepare a well-organized report based on one / all of the following:

- by attending at least 5 expert lectures/ invited talks/ Seminar/ Popular lectures etc. organized by the institute/any of the departments, ideally in a specific domain or with the same theme.
- prepare a business or marketing plan based on patent search

The student is expected to consolidate the ideas from these lectures/patent searches and may even include material from other sources to strengthen the content of the report. The student should prepare a well-organized report based on the above and present it to the panel constituted by the department, for evaluation.

Evaluation Criteria:

The student will be evaluated by the panel based on the below criteria.

Criteria	Description	Weightages
I	Clarity on the topic	15 marks
II	List of lectures attended	15 marks
III	Report	15 marks
IV	Presentation	30 marks
V	Response to questions	25 marks

Evaluation Criteria-CO Mapping

CO / Criteria	CO-1	CO-2	CO-3
I	X		
II	X		
III		X	
IV			X
V			X

CH17091 **0-0-0 (2)**

Summer Internship / Research Experience

Pre-Requisites: **None**

Course Outcomes:

CO-1	Apply engineering principles to real-world problems, gaining practical experience
CO-2	Plan, manage and execute the work with ethical consideration
CO-3	Review the social and environmental impact of the work
CO-4	Communicate the learnings through report and presentation

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	-	2	2	-	-
CO-2	3	-	2	2	3	3
CO-3	3	-	2	2	-	3
CO-4	-	3	-	-	2	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Description:

Every student has to undergo either a Summer Internship / Research project. The summer internship may be undergone in an Industry/Research organization or any premier academic Institution, including NIT Warangal for 6-8 weeks. The research project shall be registered under the guidance of any faculty member in the institute. The student is required to submit a report and present the work before an evaluation committee, nominated by the Head of the Department.

Evaluation Criteria:

The student will be evaluated by the panel based on the below criteria.

Criteria	Description	Weightages
I	Relevance of the area of work	25 marks
II	Performance of the Task	20 marks
III	Crucial learnings from the work	20 marks
IV	Report Preparation	15 marks
V	Presentation and Response to questions	20 marks

Evaluation Criteria-CO Mapping

CO / Criteria	CO-1	CO-2	CO-3	CO-4
I	X			
II		X		
III			X	
IV				X
V				X

CH17093 **0-0-0 (2)**

Comprehensive Viva-voce

Pre-Requisites: **None**

Course Outcomes:

CO-1	Comprehend the knowledge gained in the course work
CO-2	Demonstrate the ability in problem solving
CO-3	Communicate effectively using engineering terminology

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	-	2	3	3	-	3
CO-2	3	-	3	3	-	-
CO-3	-	2	3	3	-	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Description:

In Comprehensive viva-voce each student will be evaluated for their overall comprehension of the course work and laboratory training that they have undergone. The students will be expected to answer questions orally, write down simple equations, draw plots, schematics, write simple code etc. as questioned by the panel. Assessment will be done by the panel based on the student response.

CH17097 **0-0-0 (8)**

Dissertation: Part A

Pre-Requisites: None

Course Outcomes:

CO-1	Identify a topic in advanced areas of chemical engineering
CO-2	Review literature to identify gaps and define objectives and scope of the work
CO-3	Employ the ideas from literature and develop research methodology
CO-4	Develop a model, experimental set-up and / or computational techniques necessary to meet the objectives

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	-	3	-	-	-
CO-2	-	3	3	-	3	3
CO-3	-	-	2	2	3	-
CO-4	-	-	3	3	-	3

1 - Slightly; 2 - Moderately; 3 - Substantially

Description:

Students are expected to choose real-world contemporary problem and apply the engineering principles learned, to solve the problem through building prototypes or simulations or writing codes or establishing processes/synthesis/correlations etc. The department constituted panel will decide the suitability and worthiness of the Dissertation.

Dissertation Evaluation:

i. The dissertation shall be submitted as per the schedule given in the academic calendar.
ii. The dissertation supervisor will periodically review the progress of the student and finally give his/her assessment of the work done by the student.
iii. The Dissertation Part – A will be evaluated for 100 marks, with the following weightages:

Sub-component	**Weightage**
a) Periodic evaluation by Guide	40 marks
b) Mid-term review	20 marks
c) End Semester viva-voce examination	40 marks

Evaluation Criteria

The student will be evaluated by the panel based on the below criteria.

Criteria	Description	Weightages (%)
I	Selection of Topic	20
II	Literature Survey	20
III	Defining the Objectives and Solution Methodology	30
IV	Performance of the Task	30

Evaluation Criteria - CO Mapping:

CO / Criteria	CO-1	CO-2	CO-3	CO-4
I	X			
II		X		
III			X	
IV				X

Refer to M.Tech. – Regulations for any further information regarding Mid-term review, End Sem evaluation.

4th Semester

CH17098 **0-0-0 (12)**

Dissertation: Part B

Pre-Requisites: **CH1797**

Course Outcomes:

CO-1	Identify the materials and methods for carrying out experiments/develop a code
CO-2	Execute the research methodology with a concern for society, environment and ethics
CO-3	Analyse, discuss and justify the results/trends and draw valid conclusions
CO-4	Prepare the report as per recommended format and present the work orally adhering to stipulated time
CO-5	Explore the possibility to publish/present a paper in peer reviewed journals/conference proceedings without plagiarism

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	-	3	3	2	3
CO-2	-	-	3	2	3	3
CO-3	3	-	3	3	2	3
CO-4	-	3	3	-	-	-
CO-5	-	3	3	-	-	-

1 - Slightly; 2 - Moderately; 3 - Substantially

Description:

Students are expected to choose real-world contemporary problem and apply the engineering principles learned, to solve the problem through building prototypes or simulations or writing codes or establishing processes/synthesis/correlations etc. The department constituted panel will decide the suitability and worthiness of the dissertation.

Dissertation Evaluation:

i. The dissertation shall be submitted as per the schedule given in the academic calendar.
ii. The dissertation supervisor will periodically review the progress of the student and finally give his/her assessment of the work done by the student.
iii. The Dissertation Part – B will be evaluated for 100 marks, with the following weightages:

Sub-component	**Weightage**
a) Periodic evaluation by Guide	40 marks
b) Mid-term review	20 marks
c) End Semester viva-voce examination	40 marks

Evaluation Criteria:

The student will be evaluated by the panel based on the below criteria as a continuation of Dissertation Part A.

Task	Description	Weightages (%)
IV	Performance of the Task	20
V	Dissertation Preparation	25
VI	Review (Presentation & Understanding)	30
VII	Viva-Voce	15
VIII	Publications /Possibility of publication	10

Evaluation Criteria-CO Mapping:

CO / Criteria	CO-1	CO-2	CO-3	CO-4	CO-5
IV	X	X			
V				X	
VI			X		
VII				X	
VIII					X

Refer to M.Tech. – Regulations for any further information regarding Mid-term review, End Sem evaluation, Template for report preparation and plagiarism.

Professional Electives – I & II

CH16021 **3-0-0 (3)**

Circular Economy for Sustainable Development

Pre-Requisites: **None**

Course Outcomes:

CO-1	Explain the concept of circular economy and its core principles compared to the traditional linear economy
CO-2	Analyze different circular economy models (e.g., product-service systems, resource recovery, industrial symbiosis) and their applications in specific industries
CO-3	Apply circular design principles to products, processes, and systems for extending their lifespan and value retention
CO-4	Evaluate the role of policy instruments and regulations in promoting circular economy practices
CO-5	Analyze the social, economic, and environmental benefits of transitioning to a circular economy

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	2	2	-	-	1
CO-2	1	2	2	-	-	1
CO-3	1	2	2	-	-	1
CO-4	3	3	2	-	1	1
CO-5	1	3	2	-	1	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction to Circular Economy: Definition and Core Principles-The concept of circular economy and its core principles (reduce, reuse, recycle, recover); Comparison of the linear and circular economy models. Drivers and Challenges- Environmental implications of the linear economy, Drivers for transitioning to a circular economy, Challenges of implementing circular economy practices. Circular Economy and SDGs: Links between circular economy and the UN Sustainable Development Goals (SDGs).

Circular Economy Models and Applications: Circular Economy Models- Analysis of different models (e.g., circular product design, closed-loop recycling, sharing economy). Real-world examples of circular economy practices across various industries; Case Studies- Development of a case study on a company successfully implementing circular economy principles; Evaluation of the potential economic and environmental benefits of circular economy models.

Design for Circularity: Circular Design Principles- Explanation of principles (e.g., design for disassembly, durability, material selection); Application of design thinking tools for developing circular product concepts; Life Cycle Analysis- Analysis of the life cycle of a product, Identification of opportunities for circular design interventions, Comparison of Design Approaches- Comparison of traditional product design with design for circularity principles.

Policy and Governance for Circular Economy: Policy Instruments- Evaluation of the role of government policies and regulations in promoting circular economy practices; Analysis of various policy instruments used to support circularity (e.g., extended producer responsibility, eco-design regulations, taxation); Governance and Collaboration- Importance of stakeholder collaboration and multi-level governance for a

successful circular economy transition- Identification and analysis of international initiatives and frameworks promoting circular economy.

Benefits and Future of Circular Economy: Social, Economic, and Environmental Benefits- Analysis of the social, economic, and environmental benefits of a circular economy; Emerging Trends and Innovations- Discussion of emerging trends and innovations in circular economy practices; The Future of Circular Economy-Exploring the potential of circular economy for achieving sustainable development.

Learning Resources:

Text Books:

1. Walter R Stahel, The Circular Economy A User's Guide, CRC Press, 2019.
2. Peter Lacy, Jessica Long, Wesley Spindler, The Circular Economy Handbook: Realizing the Circular Advantage, Palgrave Macmillan, 2020.
3. Peter Lacy, Jakob Rutqvist, Waste to Wealth: The Circular Economy Advantage, Palgrave Macmillan, 2015.

Reference Books:

1. María-Laura Franco-García, Jorge Carlos Carpio-Aguilar, Hans Bressers, Towards Zero Waste: Circular Economy Boost, Waste to Resources, Springer International Publishing, 2019.
2. Marcello Tonelli, Nicolo Cristoni, Strategic Management and the Circular Economy, Routledge, 2018.
3. Sadhan Kumar Ghosh, Circular Economy: Global Perspective, Springer, 2020.
4. Stahel, Walter R., The Circular Economy: A User's Guide, Routledge, 2019.
5. Lerwen Liu, Seeram Ramakrishna, An Introduction to Circular Economy, Springer, 2021.

Other Suggested Readings:

1. https://online-learning.harvard.edu/course/introduction-circular-economy?delta=0

CH16023 **3-0-0 (3)**

Advanced Mass Transfer

Pre-Requisites: **None**

Course Outcomes:

CO-1	Design multicomponent columns using equilibrium-based approach
CO-2	Analyse separations involving energy and mass separating agents
CO-3	Select advanced separation technique for a given process
CO-4	Design reactive separation processes

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	-	3	3	-	1
CO-2	3	-	3	3	-	1
CO-3	3	-	3	3	-	1
CO-4	3	-	3	3	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Multi-component system fractionation: Preliminary calculations, feed condition, column pressure, design procedure, number of equilibrium stages, feed location, estimation of number of theoretical plates – shortcut methods and rigorous calculation methods.

Enhanced Distillation and Supercritical Extraction: extractive distillation, pressure-swing distillation, azeotropic distillation, reactive distillation, supercritical fluid extraction.

Membrane Separations: transport in membranes, dialysis, electrodialysis, reverse osmosis, gas permeation, pervaporation.

Adsorption, Ion Exchange, Chromatography: sorbents, equilibrium considerations, kinetic and transport considerations, equipment for sorption operations, Ion-exchange cycle.

Leaching and Washing: equipment for leaching, equilibrium-stage model for leaching and washing, rate-based model for leaching.

Reactive Separation processes: reactive distillation, extraction with reaction, absorption withreaction, adsorption with reaction, reactive membrane separation, reactive crystallization.

Learning Resources:

Text Books:

1. J.D. Seader, Ernest J. Henley, D. Keith Roper, Separation Processes Principles John Wiley& Sons, 2011, 3rd Edition.
2. King C. J., Separation Processes, Tata McGraw Hill Book Company, 1983, 2nd Edition.
3. Geankoplis C. J., Transport Processes and Unit Operations, PHI, 2004, 4th Edition.

4. Santi Kulprathipanja, Reactive Separation Processes, Taylor & Francis, 2002.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103105060

CH16025 **3-0-0 (3)**

Computational Techniques

Pre-Requisites: **None**

Course Outcomes:

CO-1	Implement linear algebra concepts for solving engineering problems
CO-2	Solve ordinary differential equations and differential algebraic equations
CO-3	Solve Partial Differential Equations
CO-4	Solve different engineering problems

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	-	3	-	-	1
CO-2	2	-	3	-	-	1
CO-3	2	-	3	-	-	1
CO-4	2	-	3	-	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Linear Algebra: Solving linear equations, Vector spaces and Subspaces, Orthogonality, Determinants, Eigenvalues and Eigen vectors, Function spaces. Cayley-Hamilton theorem, Polynomials and functions defined on matrices, Similarity transformations, Jordan forms, quadratic forms.

Linear Ordinary Differential Equations and Solution Methods.

Nonlinear Ordinary Differential Equations: Autonomous / non-autonomous systems of ODEs, Differential-Algebraic equations - Solution methods.

Partial differential equations – Solution methods for parabolic, hyperbolic and elliptic equations.

Applications to different engineering systems.

Learning Resources:

Text Books:

1. Gilbert Strang, Introduction to Liner Algebra, Wellesley-Cambridge Press, 2009, 4th Edition.
2. Gilbert Strang, Differential Equations and Linear Algebra, Wellesley-Cambridge Press, 2009.

Reference Books:

1. D W Jordan, P Smith, Nonlinear ordinary differential equations, an introduction for scientists and engineers, Oxford University Press, 2007.
2. Harumi Hattori, Partial Differential Equations: Methods, applications and Theories, World Scientific, 2019, 2nd Edition.

Other Suggested Readings:

1. http://www-math.mit.edu/~gs/index.html

CH16027 **3-0-0 (3)**

Advanced Process Modelling

Pre-Requisites: **None**

Course Outcomes:

CO-1	Differentiate model building techniques
CO-2	Develop first principle's, grey box and empirical model for a given system
CO-3	Formulate mathematical model for a process equipment
CO-4	Model discrete time systems

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	–	3	1	–	1
CO-2	2	–	3	1	–	1
CO-3	2	–	3	1	–	1
CO-4	2	–	3	1	–	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction to Modelling: a systematic approach to model building, classification of models; Conservation Principles; Constitutive Relations.

Model development: Development of steady state and dynamic, lumped and distributed parameter models based on conservation principles; Solution strategy for lumped parameter models; solution strategy for distributed parameter models; The transport phenomena models: Momentum, energy and mass transport models; Analysis of ill-conditioned systems.

Classification of systems: System's abstraction and Modelling; types of systems and examples, system variables, input-output system description, system response, analysis of system behavior, linear system, superposition principle, linearization, non-linear system analysis, system performance and performance targets.

Development of grey box models: Empirical model building; Statistical model calibration and validation; Population balance models; Examples.

Mathematical model development for different chemical engineering equipment: distillation columns, reactors, heat exchangers.

Learning Resources:

Text Books:

1. Amiya K. Jana, Chemical Process Modelling and Computer Simulation, Prentice Hall, 2011, 2nd Edition.
2. William L. Luyben, Process Modelling, Simulation and Control for Chemical Engineers, McGraw Hill Publishing Company, 1996, 2nd Edition.
3. K. M. Hangos, I. T. Cameron, Process Modelling and Model Analysis, Academic Press, 2001.

Reference Books:

1. M. Chidambaram, Mathematical Modelling and Simulation in Chemical Engineering, Cambridge University Press, 2018.
2. Ashok Kumar Verma, Process Modelling and Simulation in Chemical, Biochemical and Environmental Engineering, CRC Press, 2014.
3. Jim Caldwell, Douglas K. S. Ng, Mathematical Modelling: Case Studies, Kluwer Academic, Publishers, 2004.
4. Said S. E. H. Elnashaie, Parag Garhyan, Conservation Equations and Modelling of Chemical and Biochemical Processes, Marcel Dekker Publishers, 2003.
5. K. M. Hangos, I. T. Cameron, Process Modelling and Model Analysis, Academic Press, 2001.
6. John Ingham, Irving J. Dunn, Elmar Heinzle, J. E. Prenosil, Jonathan B. Snape, Chemical Engineering Dynamics, Wiley, 2007.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103107096

CH16029 **3-0-0 (3)**

Chemical Process Synthesis

Pre-Requisites: **None**

Course Outcomes:

CO-1	Identify the steps and information required for process synthesis
CO-2	Recognize the role of energy, environment, sustainability, safety and engineering ethics in process synthesis
CO-3	Develop preliminary process flow sheet using heuristics
CO-4	Synthesize heat exchanger networks and separation trains
CO-5	Perform economic analysis related to process design

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	3	3	2	1
CO-2	1	-	-	3	1	-
CO-3	2	2	3	3	2	1
CO-4	1	-	3	2	-	1
CO-5	-	-	3	3	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction to Process design: Preliminary Process Synthesis, Synthesis Steps, Process Design Tasks, Preliminary Flowsheet Mass Balances.

Energy, Environment, Sustainability, Safety, Engineering Ethics: Environmental Protection, Sustainability, Safety Considerations, Engineering Ethics.

Synthesis of steady state flow sheet: Introduction, Flow sheets, the problem of steady stateflow sheeting, general semantic equation of equipment, Generalization of the method of synthesis of process flow sheet, Recycle structure of the flow sheet, separation systems.

Heuristics for process synthesis: Raw materials and Chemical reactions, Distribution of chemicals, Separations, Heat exchangers and furnaces, pumping pressure reduction and conveying of solids.

Algorithmic methods for process synthesis: Synthesis of separation trains, sequencing of ordinary distillation columns, Optimization of flow sheet with respect to heat exchanger network, Network of heat exchanger, Some necessary conditions for the existence of an optimal exchanger network, Condition of optimality for the minimum area network, Rules of adjustment of the minimum heat exchanger network to find the optimal solution.

Cost Accounting and Capital Cost Estimation: Estimation of the Total Capital Investment, Purchase Costs of the Most Widely Used Process Equipment, Purchase Costs of Other Chemical Processing Equipment.

Annual Costs, Earnings, and Profitability Analysis: Annual Sales Revenues, Production Costs, and the Cost Sheet, Working Capital and Total Capital Investment, Approximate Profitability Measures, Time Value of Money, Cash Flow and Depreciation.

Learning Resources:

Text Books:

1. Seider W. D., Seader J. D., Lewin D. R., Product and Process Design Principles: Synthesis Wiley, 2016.
2. Bieglar L.T, Grossman E.I, Westerberg A.W., Systematic Methods of Chemical Process Design, Prentice Hall Inc., 1997.
3. Douglas J. M., Conceptual Design of Chemical Processes, McGraw Hill, 1988.

CH16031 **3-0-0 (3)**

Safety Analysis in Process Industries

Pre-Requisites: **None**

Course Outcomes:

CO-1	Mitigate fire and explosion hazards
CO-2	Apply hazard identification techniques
CO-3	Control reactive chemical hazards
CO-4	Implement safety aspects while designing process plants

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	–	–	2	3	2
CO-2	1	2	–	3	2	2
CO-3	2	–	2	3	1	2
CO-4	1	1	3	3	1	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Basic laboratory safety and personal protective equipment, Engineering ethics, Accident and Loss statistics, Nature of the accident process, Review of industrial accidents.

Fire and Explosion models: The fire triangle, Distinction between fires and explosions, Flammability characteristics of liquids and vapors, liquids, gases, and vapors, Vapor mixtures, Flammability limit dependence on temperature, Flammability limit dependence on pressure, Estimating flammability limits, Limiting oxygen concentration and inerting, Flammability diagram, Ignition energy, Auto ignition, Auto-Oxidation, Adiabatic compression, Ignition sources, Sprays and Mists, Explosions, Detonation and Deflagration.

Electrical Safety Hazard: Electrical hazards, Fundamentals of electrical hazards, Fundamentals of electricity, Electrical shock, Control of electrical hazards.

Hazard identification Techniques: Non-scenario based: Checklist analysis, safety review, relative ranking, preliminary hazard analysis (PHA), fire explosion and toxicity index (FETI); Scenario based: Fault Tree Analysis & Event Tree Analysis, Logic symbols, methodology, minimal cut set ranking –various indices –what-if analysis/checklist analysis-hazard operability studies (HAZOP) -Hazard Analysis (HAZAN) -Failure Mode and Effect Analysis (FMEA).

Safety in Process industries: Chemical process industries-Requirements and Government regulations, Hazards associated with process, Decomposition & Runaway reactions, Fault tree analysis of batch reactor, Reactive chemical hazard, Decomposition energy, Hazardous unit processes, Hazards associated with exothermic reaction–case studies, Fault tree of reactor overpressure, Components of intrinsic safety, Assessing reaction hazard, Steps to reduce reactive hazards, Controlling reactive hazards.

Safety Aspects in Process Plant Design: Process plant safety, Chemical plant design, Flow diagrams, Piping and Instrumentation Diagram/Drawing (P&ID), Control system, Alarms in processes, Equipment and Piping, Chemical plant layout, Active fire protection, Emergency shutdown system, Pressure vessel design, Standards and codes-pipe works and valves heat exchangers-process machinery-over pressure protection,

Pressure relief devices and design, Fire relief, Vacuum and thermal relief, Special situations, Disposal-flare and vent systems failures in pressure system.

Learning Resources:

Text Books:

1. Frank P. Lees, Loss Prevention in Process Industries: Hazard Identification, Assessment and Control, Butterworth-Heinemann Ltd, 1996, 2nd Edition.
2. D. A. Crowl, J.F. Louvar, Chemical Process Safety (Fundamentals with Applications), Prentice Hall, 2019, 4th Edition.

Reference Books:

1. Accident Prevention Manual for Industrial Operations, National Safety Council, 1982.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103107156
2. https://nptel.ac.in/courses/110105094
3. U.S Chemical Safety Board (www.csb.gov)

CH16033 **3-0-0 (3)**

Green and Cleaner Technologies

Pre-Requisites: **None**

Course Outcomes:

CO-1	Estimate the carbon credits of various activities
CO-2	Apply principles of energy efficient technologies
CO-3	Understand the importance of green fuels and its impact on environment
CO-4	Identify the importance of life cycle assessment

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	1	1	1	1
CO-2	2	2	1	2	1	1
CO-3	2	2	3	3	–	1
CO-4	2	1	3	3	1	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Greenhouse Emissions & Carbon Accounting: climate change and role of green and cleaner technologies, causes and effects. Diagnostics and baseline determination, climate change mitigation and adaptation strategy. Risk assessments & mitigation, carbon market, carbon capture and storage, potential carbon sequestration (forest sinks).

Green Technology: definition, Importance, historical evolution, advantages and disadvantages of green technologies, factors affecting green technologies, role of Industry, government and institutions, industrial ecology, role of industrial ecology in green technology.

Principles of Green Technologies: reasons for Green Technology, resource minimization, waste minimization, concepts, green reactions solvent free reactions, catalyzed (heterogeneous/homogeneous) reactions, ultrasound mediated reactions, bio catalysts etc.

Materials for "Green" Systems: Green materials, including biomaterials, biopolymers, bioplastics, and composites. Green technologies for energy, green fuels, definition, benefits and challenges, comparison of green fuels with conventional fossil fuels with reference to environmental, economic and social impacts. Various technologies available for energy production- Wind, solar biofuels etc.

Principles of Cleaner Production: Barriers, role of Industry, clean development mechanism, reuse, recovery, recycle, raw material substitution, wealth from waste, case studies. Over view of cleaner production assessment steps and skills, process flow diagram, material balance, cleaner production, option generation, technical and environmental feasibility analysis, economic valuation of alternatives.

Learning Resources:

Text Books:

1. Clark, J.H., Macquarrie, D.J., Handbook of Green Chemistry and Technology, John Wiley and Sons, 2002.

2. Paul Anastas, John Warner, Green Chemistry: Theory and Practice, Oxford University Press, 2000.
3. Mike Lancaster, Green Chemistry- An introductory Text, Royal Society of Chemistry, 2016, 3rd Edition.

Reference Books:

1. Matthew N. O. Sadiku, Emerging green technologies, CRC Press, 2020.
2. Pradeep Tomar, Gurjit Kaur, Green and Smart Technologies for Smart Cities, CRC Press, 2019.

CH16035 **3-0-0 (3)**

Industrial Instrumentation

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand techniques for measurement of level, pressure
CO-2	Measure temperature using contact / non-contact techniques
CO-3	Analyze methods for torque and velocity
CO-4	Select methods for acceleration, vibration and density measurement
CO-5	Identify a suitable technique for flow measurement

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	-	1	-	-	1
CO-2	2	-	1	-	-	1
CO-3	2	-	1	-	-	1
CO-4	2	-	1	-	-	1
CO-5	2	-	1	-	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Level measurement: Gauge glass technique coupled with photo electric read out system, float type level indication, different schemes, measurement using displacer and torque tube – bubbler system. Differential pressure method. Electrical types of level gauges using resistance,capacitance, nuclear radiation and ultrasonic sensors.

Pressure measurement: Manometers, pressure gauges – Bourde type bellows, diaphragms. Electrical methods – elastic elements with LVDT and strain gauges. Capacitive type pressuregauges. Measurement of vacuum – McLeod gauge – thermal conductivity gauges – Ionization gauge cold cathode and hot cathode types – testing and calibration.

Temperature measurement: Thermometers, different types of filled in system thermometer, bimetallic thermometers. Electrical methods, signal conditioning of industrial RTDs and their characteristics –3 lead and 4 lead RTDs. Thermocouples and pyrometers.

Flow measurement: Volumetric flow measurement through electromagnetic, ultrasonic and vortex techniques. Mass flow measurement through Coriolis Principle. Basics of analyzers - single and multiple components through chromatography. Control valves – different types, characteristics and smart valves.

Measurement of force torque, velocity: Electric balance – different types of load cells – magnets – elastics load cell-strain gauge load cell. Different methods of torque measurement,strain gauge, relative regular twist-speed measurement- revaluation counter- capacitive tacho-drag up type tacho D.C and A.C tacho-generators – stroboscope.

Measurement of acceleration, vibration and density: Accelerometers – LVDT, piezo- electric, strain gauge and variable reluctance type accelerometers, calibration of vibration pickups, Baume scale API scale, pressure head type densitometer, float type densitometer.

Learning Resources:

Text Books:

1. William C. Dunn, Fundamentals of Industrial Instrumentation and Process Control, McGraw Hill, 2005.
2. R. K. Jain, Mechanical and Industrial Measurements, Khanna Publishers, 1999
3. E. L. Upp, Paul J. LaNasa, Fluid Flow Measurement, Gulf Professional Publishers, 2002, 2nd Edition.

Reference Books:

1. Bela G. Liptak, Instruments Engineers Handbook, CRC Press, 2003, 4th Edition.
2. D. Patranabis, Principles of Industrial Instrumentation, Tata McGraw Hill, 1999.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103105130

CH16037 **3-0-0 (3)**

Solid Waste Management

Pre-Requisites: **None**

Course Outcomes:

CO-1	Identify various types of solid wastes and their sources
CO-2	Examine the physical and chemical composition of wastes
CO-3	Analyze the activities associated with the management of solid waste
CO-4	Evaluate the techniques and methods used in the recovery of materials and energy from solid wastes
CO-5	Design a sanitary landfill for disposal of solid waste
CO-6	Categorize and manage hazardous waste

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	-	1	2	1	1
CO-2	2	-	1	3	1	1
CO-3	2	-	1	2	-	1
CO-4	2	-	1	3	1	1
CO-5	2	-	1	3	1	1
CO-6	2		1	2	1	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Solid Waste: Definitions, Characteristics, and Perspectives: Types of solid wastes, sources of solid wastes, properties of solid wastes, solid waste management: an overview.

Engineering Systems for Solid Waste Management: Solid waste generation; on-site handling, storage, and processing; collection of solid wastes; transfer and transport; processing techniques; ultimate disposal; Integrated SW Management concepts.

Engineering Systems for Resource and Energy Recovery: Processing techniques; RRR approach, materials-recovery systems; recovery of biological conversion products; recovery ofthermal conversion products; recovery of energy from conversion products; materials and energy recovery systems.

Engineering Disposal of SW: Dumping of solid waste; sanitary landfills—site selection, design, and operation of sanitary landfills—leachate collection and treatment. Identify solid waste disposal methods during a site visit and follow safety precautions.

Hazardous Waste Management: Introduction; Concern about Hazardous Waste Management; Characteristics of Hazardous Waste; Transportation and Disposal of Hazardous Waste; Industrial/biomedical waste, E- waste management.

Learning Resources:

Text Books:

1. Tchobanoglous G., Theisen H., Vigil S.A., Integrated Solid Waste Management, Engineering Principles and Management Issues, McGraw Hill, 2014.
2. John Pichtel, Waste Management Practices: Municipal, Hazardous and Industrial, CRCPress, 2014, 2nd Edition.
3. Vesilind P.A., Worrell W., Reinhart D., Solid Waste Engineering, Brooks/Cole Thomson Learning Inc., 2010, 2nd Edition.

Reference Books:

1. Peavy, H.S, Rowe, D.R., G. Tchobanoglous, Environmental Engineering, McGraw Hill, 2017, 1st Edition.
2. Tchobanoglous G., Kreith F., Handbook of Solid Waste Management, McGraw Hill, 2002, 2nd Edition.
3. Qian X., Koerner R.M., Gray D.H., Geotechnical Aspects of Landfill Design and Construction, Prentice Hall, 2002, 1st Edition.
4. LaGrega M.D., Buckingham P.L., Evans J.C., Hazardous Waste Management, Waveland Pr Inc., 2010.
5. Richard J. Watts, Hazardous Wastes - Sources, Pathways, Receptors, John Wiley and Sons, 1998, 1st Edition.

Other Suggested Readings:

1. http://cpheeo.gov.in/cms/manual-on-municipal-solid-waste-management-2016.php
2. https://nptel.ac.in/courses/105103205
3. https://nptel.ac.in/courses/120108005
4. https://nptel.ac.in/courses/105106056
5. https://nptel.ac.in/courses/105105160
6. https://nptel.ac.in/courses/103107125

CH26001 **3-0-0 (3)**

Sustainable Energy Engineering

Pre-Requisites: **None**

Course Outcomes:

CO-1	Quantify the variety of energy resources
CO-2	Perform project economics evaluation
CO-3	Evaluate sustainability metrics
CO-4	Select suitable sustainable energy technologies

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	1	3	3	2	1
CO-2	1	2	2	2	3	1
CO-3	2	2	2	2	3	1
CO-4	1	2	2	3	2	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Sustainability Concepts: Sustainable Development Goals for Clean Energy (SDGS), Emerging Issues in Energy Access, Technologies, Economics. Sustainability Concepts of Energy Generation Technologies, Energy and Resource Utilization.

Sustainable Energy: The Engine of Sustainable Development: Aspects of Energy Production, Nations and Global Patterns of Energy Supply and Utilisation, Environmental Effects of Energy.

Estimation and Evaluation of Energy Resources: Comparison of Different Forms of Energy, Energy Life Cycle, Estimation and Validation of Energy Resources.

Technical Performance: Allowability, Efficiency, Production Rates, Relation of Technical Performance to Sustainability, Thermodynamic Analysis, Chemical Rate Processes, Use and Abuse of Time Scales.

Local, Regional, and Global Environmental Effects of Energy: Adverse Environmental Effects, Attribution of Environmental Damage, Methods of Environmental Protection.

Project Economic Evaluation: Time Value of Money Mechanics, Economy of Scale and Learning Curve, Energy Accounting.

Energy Systems and Sustainability Metrics: System Analysis Approach, Measures, General Principles for Sustainable Development.

Energy, Water and Land Use: Major Planetary Cycles, Land-Use Issues, Ocean-Use Issues, Implications for Sustainable Energy, Charting Pathways for Energy Democracy, Building an Energy Democracy Movement.

Biomass Energy, Biofuel: Characterization, Biomass Relevance to Energy Production, Properties Relevant to Energy Production, Thermal Conversion, Bioconversion, Economics.

Solar Energy: Resource Assessment, Concentrating Solar Power, Solar Photovoltaic Systems.

Ocean Wave, Tide, Current, and Thermal Energy Conversion: Energy from the Tides and Currents, Energy from Waves, Economic Prospects, Environmental and Sustainability Considerations.

Wind Energy: Wind Resources, Wind Machinery and Generating Systems, Wind Power Economics, Measure of Sustainability.

Energy Carriers: Electric Power, Hydrogen Fuel: Electricity as an Energy Carrier, Hydrogen as an Energy Carrier, Sustainability Issues.

Industrial Energy Usage: Life-Cycle Analysis and Design for Sustainability, Chemical Industries, Cement and Lime Industries, Sustainability Issues.

Synergistic Complex Systems: Complex Systems View, Some Case Studies, Transitional Pathways, Challenge to Society.

Learning Resources:

Text Books:

1. Tester J. W., Drake E. M., Driscoll M. J., Golay M. W., Peters W. A., Sustainable Energy: Choosing Among Options, Tester, MIT Press, 2012, 2nd Edition.
2. Martin A. Abraham, Encyclopedia of Sustainable Technologies, Elsevier Publications, 2024, 2nd Edition.
3. Eduardo Rincon-Mejia, Alejandro de las Heras, Sustainable Energy Technologies, CRC Press, Taylor & Francis Group, 2018.
4. Denise Fairchild, A.l. Weinrub, Energy democracy: Advancing equity in clean energy solutions, Island press, 2017

Reference Books:

1. Mulligan C. N., Sustainable Engineering: Principles and Implementation, CRC Press,Taylor and Francis Group, 2019.
2. Bakshi B. R., Sustainable Engineering: Principles and Practice, Cambridge UniversityPress, 2019.
3. David Allen, David Shonnard, Sustainable Engineering: Concepts, Design, and Case Studies, Prentice Hall, 2011.
4. Hazra Somnath, Bhukta Anindya,Sustainable Development Goals an Indian Perspective, Springer, 2020.

CH26003 **3-0-0 (3)**

Hydrogen Generation and Storage

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the basic properties of hydrogen, including its chemical and physical characteristics, and its role as an energy carrier
CO-2	Select a suitable hydrogen generation and storage technique based on the mechanisms, performance characteristics, and applicability
CO-3	List the safety considerations and regulations related to hydrogen handling
CO-4	Analyze the economic viability and environmental impact of hydrogen generation and storage systems

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	1	1	1	1	1
CO-2	1	1	1	1	2	1
CO-3	1	1	2	2	1	1
CO-4	1	1	2	2	2	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Basic Properties of Hydrogen; Engineering Thermodynamics; Hydrogen and Environment; Hydrogen and Sustainability; Hydrogen Production Methods; Green Hydrogen Sources; Hydrogen as an Energy Carrier; Historical Background and Current Applications.

Hydrogen Generation Methods: Steam methane reforming; Electrolysis (alkaline; PEM, and solid oxide electrolysis); Coal/Biomass Gasification; Solar and Wind-based Hydrogen Production; Emerging Hydrogen Generation Technologies.

Hydrogen Storage Techniques: Compressed Gas Storage; Liquid Hydrogen Storage; Chemical Storage (hydrogenation, metal hydrides); Physical Storage Using Nanostructured and Porous Materials; Underground Hydrogen Storage; Emerging Hydrogen Storage Technologies.

Performance and Efficiency: Efficiency Considerations in Hydrogen Generation; Energy Losses and Efficiency of Different Storage Methods; Performance Assessment of Hydrogen Production and Storage Systems.

Safety and Regulations: Safety Considerations in Hydrogen Handling and Storage; Codes and Standards for Hydrogen Storage Systems; Risk Assessment and Mitigation Strategies; Case Studies of Hydrogen-related Incidents.

Learning Resources:

Text Books:

1. Gupta, R. B., Hydrogen Fuel: Production, Transport, and Storage, CRC press, 2008.

2. Zhang, J. Z., Li, J., Li, Y., Zhao, Y., Hydrogen Generation, Storage and Utilization, John Wiley & Sons, 2014.
3. Dinçer, I., Zamfirescu, C., Sustainable Hydrogen Production, Elsevier, 2016.

Reference Books:

1. Altalhi, T. A., Adnan, S. M., Amin, M. A., Materials for Hydrogen Production, Conversion, and Storage, John Wiley & Sons, 2023.
2. Winter, C. J., Nitsch, J., Hydrogen as an Energy Carrier: Technologies, Systems, Economy, Springer Science & Business Media, 2012.
3. Sherif, S. A., Goswami, D. Y., Stefanakos, E. L., Steinfeld, A., Handbook of Hydrogen Energy, CRC press, 2014.

Other Suggested Readings:

1. https://onlinecourses.nptel.ac.in/noc22_ch66/preview

CH26021 **3-0-0 (3)**

Fuel Cell Systems

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand working principle of fuel cell
CO-2	Analyse the performance of fuel cell systems
CO-3	Identify the intricacies in the operation of fuel cell stack and fuel cell system
CO-4	Analyse the fuel cell system design and integration

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	2	3	2	1	1
CO-2	1	2	3	2	1	1
CO-3	1	2	3	2	2	1
CO-4	2	2	3	2	1	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction to Fuel Cells: Fuel Cells as Electrochemical Engines; Generic Fuel Cell and Stack; Classification of Fuel Cells; Potential Applications; History of Fuel Cell Development.

Thermodynamics and Basic Electrochemical Principles: Heat; Work Potentials; Prediction of Theoretical Voltage, Fuel Cell Efficiency; Electrode Kinetics; Butler-Volmer Equation; Overpotentials; Tafel Equation; Exchange Currents.

Fuel Cell Components and Their Impact on Performance: Fuel Cell Performance Characteristics – Current/Voltage; Voltage Efficiency and Power Density; Ohmic Resistance; Kinetic Performance; Membrane Electrode Assembly Components; Fuel Cell Stack; Bi-Polar Plate; Humidifiers and Cooling Plates.

Principles and technology of different types of fuel cell systems: Alkaline Fuel Cells; Molten Carbonate Fuel Cells; PEM Fuel Cells; Solid Oxide Fuel Cells; Phosphoric acid Fuel Cells; Microbial Fuel Cells; Regenerative Fuel Cells.

Fuel Cell System Design and Testing: Performance Testing and Measurement Techniques; Electrochemical and Physical Characterization Techniques; Thermal Management and Water Management; Hydrogen Production from Renewable Sources and Storage; Safety Issues; Cost Analysis.

Learning Resources:

Text Books:

1. Hoogers G , Fuel Cell Technology Hand Book, CRC Press, 2003, 1st Edition.
2. Mathew M. Mench, Fuel Cell Engines, Wiley, 2008, 1st Edition.
3. O'Hayre, R. P., Cha, S., Colella, W., Prinz, F. B., Fuel Cell Fundamentals, Wiley, 2016, 3rd Edition.
4. Barbir, F., PEM Fuel Cells: Theory and Practice, Elsevier, 2013, 2nd Edition.

Reference Books:

1. Detlef Stolten, Bernd Emonts , Fuel Cell Science and Engineering – Materials, Processes, Systems and Technology, Vol-1, Wiley-VCH, 2012, 1st Edition.
2. Subhash C. Singal, Kevin Kendall, High Temperature Fuel Cells: Fundamentals, Design and Applications, Elsevier Science, 1985, 1st Edition.
3. Laminie, J., Dicks, A., John Wiley, Fuel Cell Systems Explained, New York, 2003, 2nd Edition.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103102015

CH26027 **3-0-0 (3)**

Waste to Energy

Pre-Requisites: **None**

Course Outcomes:

CO-1	Demonstrate technologies for generation of energy from solid waste
CO-2	Select thermochemical conversion methods
CO-3	Identify sources of energy from biochemical conversion
CO-4	Analyse the environmental and health impact of waste to energy conversion

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	-	1	1	1
CO-2	2	2	-	1	2	1
CO-3	2	2	-	1	-	1
CO-4	2	1	-	2	2	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Characterization of Wastes, Agricultural Residues and Wastes Including Animal Wastes, Industrial Wastes, Municipal Solid Wastes. Waste Processing Types and Composition of Various Types of Wastes, Characterization of Municipal Solid Waste, Industrial Waste and Biomedical Waste, Waste Collection and Transportation, Waste Processing-Size Reduction, Separation, Waste Management Hierarchy, Waste Minimization and Recycling of Municipal Solid Waste.

Thermochemical Conversion: Incineration, Pyrolysis, Gasification of Waste Using Gasifiers, Environmental and Health Impacts of Incineration; Strategies for Reducing Environmental Impacts. Energy Production from Wastes Through Incineration, Energy Production Through Gasification of Wastes. Energy Production Through Pyrolysis and Gasification of Wastes, Syngas Utilization.

Biochemical Conversion: Anaerobic Digestion of Sewage and Municipal Wastes, Direct Combustion of MSW-Refuse Derived Solid Fuel, Industrial Waste, Agro Residues, Anaerobic Digestion Biogas Production, and Present Status of Technologies for Conversion of Waste into Energy, Design of Waste to Energy Plants for Cities, Small Townships and Villages, Energy Production from Wastes Through Fermentation and Trans Esterification, Cultivation of Algal Biomass from Wastewater and Energy Production from Algae, Energy Production from OrganicWastes Through Anaerobic Digestion and Fermentation, Introduction to Microbial Fuel Cells, Process Analysis and Reactor Configurations for Methane Production, Energy Assessment, Bio-Methanation from Sludge Digestion.

Energy Production from Waste Plastics, Gas Cleanup Waste, Heat Recovery: Concept of Conversion Efficiency, Energy Waste, Waste Heat Recovery Classification, Advantages and Applications, Commercially Viable Waste Heat Recovery Devices.

Environmental and Health Impacts-Case Studies: Environmental and Health Impacts of Waste to Energy Conversion, Case Studies of Commercial Waste to Energy Plants, Waste to Energy- Potentials and Constraints in India, Eco-Technological Alternatives for Waste to Energy Conversions.

Learning Resources:

Text Books:

1. Robert C. Brown, Thermo-chemical Processing of Biomass: Conversion into Fuels, Chemicals and Power, John Wiley and Sons, 2019.
2. Sergio Capareda, Introduction to Biomass Energy Conversions, CRC Press, 2013.
3. Krzysztof J Ptasinski, Efficiency of Biomass Energy: An Exergy Approach to Biofuels, Power and Biorefineries, John Wiley & Sons, 2016.
4. Vesilind, P. A., Worrell W. A., Solid Waste Engineering, Cengage India, 2016, 2nd Edition.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103107125

Professional Electives – III, IV & V

CH16022 **3-0-0 (3)**

Wastewater Treatment

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the principles and operation of wastewater treatment systems
CO-2	Identify suitable treatment processes
CO-3	Evaluate process operations and performance
CO-4	Differentiate coagulation, flocculation, sedimentation, filtration and disinfection

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	1	1	-	1
CO-2	2	2	1	2	-	1
CO-3	2	2	3	3	-	1
CO-4	2	1	3	3	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Sources of wastewater; Necessity of treatment; Critical wastewater quality parameters; Water quality guidelines and standards for various water uses; Wastewater flowrates and constituent loadings.

Wastewater microbiology: Bacteria; Cell composition and structure; Bacterial growth curve; Classification by carbon and energy requirement; Classification by oxygen requirement; Classification by temperature, Bacteria of significance – Archaea, Protozoa, Algae, Fungi, Virus.

Classification of wastewater treatment methods: Physical treatment; Chemical treatment; Biological treatment; Levels of wastewater treatment: Preliminary treatment, Primary treatment, Enhanced primary treatment, Conventional secondary treatment, Secondary treatment with nutrient removal, Tertiary treatment, Advanced treatment.

Preliminary treatment: Screens; Shredder/grinder; Grit chambers; Primary treatment - Types of settling/sedimentation, Primary sedimentation, Chemically enhanced primary treatment.

Secondary treatment (Suspended growth processes): Microbial growth kinetics; Activated sludge process; Aeration requirements; Types of aerators; Types of suspended growth processes; Staged activated sludge process; Extended aeration process; Oxidation ditch; Sequencing batch reactor (SBR); Membrane biological reactor (MBR); Stabilization ponds and lagoons.

Secondary treatment (Attached growth and combined processes): System microbiology and biofilms; Stone media trickling filter; Rotating biological contactor; Hybrid processes; Moving bed biofilm reactor (MBBR); Integrated fixed-film activated sludge (IFAS); Fluidized bed bioreactor (FBBR); Combined processes.

Secondary Clarification: Secondary clarifier for attached growth processes and suspended growth processes.

Anaerobic wastewater treatment: Anaerobic growth kinetics; Anaerobic attached and suspended growth processes.

Solids processing and disposal: Characteristics of municipal sludge; Sludge thickening and stabilization; Biosolids dewatering.

Introduction to advanced treatment processes: Membrane processes; Ceramic and polymeric membrane processes; Microfiltration; Ultrafiltration, Reverse osmosis.

Learning Resources:

Text Books:

1. MetCalf, Eddy, Wastewater engineering, Treatment and Reuse, Tata McGraw Hill, 2003, 3rd Edition.
2. Rumana Riffat, Fundamentals of Wastewater Treatment and Engineering, CRC Press, 2013.

Reference Books:

1. S.J. Arceivala, S.R. Asolekar, Wastewater Treatment for Pollution Control and Reuse, Tata McGraw Hill, 2007, 3rd Edition.
2. Fair, G.M., Geyer J.C, Okun, Water and Wastewater Engineering, John Wiley Publications, 2010, 3rd Edition.
3. Tchobanoglous G., Burton F. L., Stensel H.D., Wastewater Engineering: Treatment and Reuse, Tata McGraw Hill, 2002, 4th Edition.

Other Suggested Readings:

1. https://onlinecourses.nptel.ac.in/noc19_ce32/preview

CH16024 **3-0-0 (3)**

Engineering Optimization

Pre-Requisites: **None**

Course Outcomes:

CO-1	Formulate objective function for a given problem
CO-2	Solve unconstrained single and multi-variable optimization problems
CO-3	Apply linear programming and nonlinear programming techniques
CO-4	Use dynamic programming for optimization

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	-	2	-	-	1
CO-2	3	-	2	-	-	1
CO-3	3	-	2	-	-	1
CO-4	3	-	2	-	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

The Nature and Organization of Optimization Problems: What Optimization is all about, Why Optimize? Scope and Hierarchy of Optimization, Examples of applications of Optimization,The Essential Features of Optimization Problems, General Procedure for Solving Optimization Problems, Obstacles to Optimization.

Basic Concepts of Optimization: Continuity of Functions, Unimodal vs multimodal functions,Convex and concave functions, convex region, Necessary and Sufficient Conditions for an Extremum of an Unconstrained Function, Interpretation of the Objective Function in terms of its Quadratic Approximation.

Optimization of Unconstrained Functions: One Dimensional search Numerical Methods for Optimizing a Function of One Variable, Scanning and Bracketing Procedures, Newton and Quasi-Newton Methods of Unidimensional Search, Polynomial approximation methods, How One-Dimensional Search is applied in a Multidimensional Problem, Evaluation of Unidimensional Search Methods.

Unconstrained Multivariable Optimization: Direct methods, Indirect methods – first order, Indirect methods – second order.

Linear Programming and Applications: Basic concepts in linear programming, Degenerate LP's – Graphical Solution, Natural occurrence of Linear constraints, The Simplex methods of solving linear programming problems, standard LP form, Obtaining a first feasible solution, Sensitivity analysis, Duality in linear programming.

Nonlinear programming with constraints: The Lagrange multiplier method, Necessary and sufficient conditions for a local minimum, introduction to quadratic programming.

Optimization of Staged and Discrete Processes: Dynamic programming, Introduction to integer and mixed integer programming, Assignment problem (Hungarian method).

Learning Resources:

Text Books:

1. Edgar T.F., D. M. Himmelblau, Optimization of Chemical Processes, McGraw Hill, 2001, 2nd Edition.
2. Stoecker W. F., Design of Thermal Systems, McGraw Hill, 2011, 3rd Edition.

Reference Books:

1. Singiresu S Rao, Engineering Optimization: Theory and Practice, John Wiley & Sons Ltd., 2019, 5th Edition.
2. Stephen Boyd, Lieven Vandenberghe, Convex optimization, Cambridge University Press, 2004.
3. P. Venkataraman, Applied Optimization with MATLAB Programming, Wiley, 2009, 2nd Edition

Other Suggested Readings:

1. https://archive.nptel.ac.in/courses/103/105/103105139/

CH16026 **3-0-0 (3)**

CO_2 Capture, Sequestration and Utilization

Pre-Requisites: **None**

Course Outcomes:

CO-1	Identify the necessity of CO_2 capture, storage and utilization
CO-2	Distinguish the CO_2 capture techniques
CO-3	Evaluate CO_2 storage and sequestration methods
CO-4	Assess environmental impact of CO_2 capture and utilization

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	2	1	1	1	2
CO-2	3	2	1	1	1	2
CO-3	3	2	2	1	1	2
CO-4	3	2	1	3	1	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Global Status of CO_2 Emission Trends; Policy and Regulatory Interventions in Abatement of Carbon Footprint; Carbon Capture, Storage and Utilization (CCS&U).

CO_2 Capture Technologies from Power Plants: Post-Combustion Capture; Pre-Combustion Capture; Oxy-Fuel Combustion; Chemical Looping Combustion; Calcium Looping Combustion.

CO_2 Capture Agents and Processes: Capture Processes; CO_2 Capture Agents; Adsorption; Ionic Liquids; Metal Organic Frameworks.

CO_2 Storage and Sequestration: Geological Sequestration Methods; Biomimetic Carbon Sequestration.

CO_2 Utilization: CO_2 Derived Fuels for Energy Storage; Polymers from CO_2; CO_2 Based Solvents; CO_2 to Oxygenated Organics; Conversion into Higher Carbon Fuels; High Temperature Catalysis.

Environmental Assessment of CO_2 Capture and Utilization: Need for Assessment; Green Chemistry and Environmental Assessment Tools; Life Cycle Assessment (LCA); ISO Standardization of LCA; Method of Conducting an LCA for CO_2 Capture and Utilization.

Learning Resources:

Text Books:

1. Peter Styring, Elsje Alessandra Quadrelli, Katy Armstrong, Carbon dioxide Utilization: Closing the Carbon Cycle, Elsevier, 2015.
2. Goel, M., Sudhakar, M., Shahi, R. V., Carbon Capture, Storage and, Utilization: A Possible Climate Change Solution for Energy Industry, TERI, Energy and Resources Institute, 2015.
3. Amitava Bandyopadhyay, Carbon Capture and Storage, CO_2 Management Technologies, CRC Press, 2014.

Reference Books:

1. Fennell, P., Anthony, B., Calcium and Chemical Looping Technology for Power Generation and Carbon Dioxide (CO_2) Capture, Woodhead Publishing Series in Energy: No. 82, 2015.
2. Mercedes Maroto-Valer M., Developments in Innovation in Carbon Dioxide Capture and Storage Technology: Carbon Dioxide Storage and Utilization, Woodhead Publishing Series in Energy, 2014, Vol 2.
3. Alireza Bahadori, Fundamentals of Enhanced Oil and Gas Recovery from Conventional and Unconventional Reservoirs, Elsevier, 2018.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103/107/103107157/
2. https://climate.mit.edu/explainers/carbon-capture

CH16028 **3-0-0 (3)**

Energy Audit and Conservation

Pre-Requisites: **None**

Course Outcomes:

CO-1	Implement energy audit for a process plant
CO-2	Plan energy conservation strategies
CO-3	Evaluate the suitability of renewable energy resources
CO-4	Analyze the energy utilization of a process equipment

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	2	1	3	1	1
CO-2	3	2	2	3	-	-
CO-3	3	1	1	3	-	-
CO-4	3	1	1	3	-	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Energy Scenario: Energy use patterns, energy resources, Oil - a critical resource, economic and environmental consideration, Future scenario.

Heat & work: First & Second law of thermodynamics, Heat Engines.

Energy Audit: Energy conversion, Energy index, Energy consumption representation - pie chart, Sankey diagram & load profile, general audit, detailed audit, waste heat recovery.

Targeting and Conservation: Energy utilization and conversion – thermal efficiency, Heat Exchangers – heat recovery, Air conditioners – supply and removal of heat.

Use of alternate energy: Solar energy, Wind energy, Nuclear energy, Biomass, Geothermal energy, Future Energy Alternatives.

Energy Integration: Pinch Analysis and Process Heat Integration, Energy Management, Key Performance Indicators and Energy Dashboards.

Case Studies: Energy conservation in alcohol industry, fertilizer industry, and pulp and paper industry, Energy conservation in different units of refinery like FCCU, HCU and ADU.

Learning Resources:

Text Books:

1. Murphy W.R. and Mckay G., Energy Management, Elsevier, 2007.
2. Hinrichs R. A. and Kleinbach M. H., Energy: Its Use and the Environment, Cengage Learning, 2012.

3. Capehart B. L., Turner W. C. and Kennedy W. J.,Guide to Energy Management, Keinnedu Fairmant press, 2011, 7th Edition.

Reference Books:

1. Rai G. D., Non-conventional Energy Sources, Khanna Publishers, 2010.
2. A.P Rossiter, B.P Jones, Energy Management and Efficiency for the process industries, Wiley, 2015.

Other Suggested Readings:

1. https://nptel.ac.in/courses/112105221

CH16030 **3-0-0 (3)**

Novel Separation Techniques

Pre-Requisites: **None**

Course Outcomes:

CO-1	Select a membrane and membrane process for a given application
CO-2	Evaluate the flux of solvent and solute through membrane
CO-3	Differentiate surfactant based separation
CO-4	Design centrifugal separation processes

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	-	2	1	-	1
CO-2	1	-	2	3	-	1
CO-3	1	-	2	3	-	1
CO-4	1	-	2	2	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Fundamentals of separation processes, basic definitions of relevant terms.

Membrane separation process: Definition of Membrane, Membrane types, Advantages and limitations of membrane technology compared to other separation processes, Membrane materials and properties.

Preparation of synthetic membranes: Phase inversion membranes, Preparation techniques for immersion precipitation, Synthesis of asymmetric and composite membranes and Synthesisof inorganic membranes.

Transport in membranes: Introduction, Driving forces, Non-equilibrium thermodynamics, Transport through porous membranes, transport through non-porous membranes, Transport through ion-exchange membranes.

Membrane processes: Pressure driven membrane processes, Concentration as driving force, electrically driven membrane processes.

Polarization phenomena and fouling: Concentration polarization, Pressure drop, Membrane fouling, methods to reduce fouling.

Modules: Introduction, membrane modules, Comparison of the module configurations.

Gas separation: Basic Principles, Membranes for gas separations, membrane modules, gas transport mechanisms, factors affecting gas permeation, complete mixing model, cross flow model, counter current model.

Surfactant based separation processes: Liquid membranes: Fundamentals and modelling, Micellar enhanced separation processes, Cloud point extraction.

Other separation processes: Centrifugal Separation processes and their calculations, Ion exchange and chromatographic separation processes,Supercritical fluid extraction.

Learning Resources:

Text Books:

1. Mulder M, Basic Principles of Membrane Technology, Kluwer Academic Publishers, 1996.
2. Baker R.W., Membrane Technology and Research, Inc. (MTR), 2004.
3. Nath K., Membrane Separation Processes, Prentice-Hall Publications, 2008.
4. R.W. Rousseau, Handbook of Separation Process Technology, John Wiley & Sons, 1987.
5. McHugh, M.A., Krukonis, V.J., Supercritical Fluid Extraction: Principles and Practice, Butterworth-Heinemann, 1994, 2nd Edition.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103105060

CH16032 **3-0-0 (3)**

Characterization Techniques

Pre-Requisites: **None**

Course Outcomes:

CO-1	Apply appropriate characterization technique for microstructure and compositional analysis of materials
CO-2	Select suitable microscope for morphology and microstructure investigation
CO-3	Analyse the crystal structure of a given material using diffraction data
CO-4	Analyse thermal stability and thermodynamic transitions of the materials

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	2	-	3	1	1
CO-2	3	2	-	3	1	1
CO-3	3	2	-	3	1	1
CO-4	3	2	-	3	1	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: materials and material characterization techniques & need of material characterization.

Microscopy: Optical microscope - Basic principles and components, Different examination modes. Electron microscopy: Interaction of electrons with solids, Scanning electron microscopy, Transmission electron microscopy and specimen preparation techniques, Scanning transmission electron microscopy.

Surface Analysis: Atomic force microscopy, Scanning probe microscopy and X-ray photoelectron spectroscopy.

Spectroscopy: Fourier transform infrared spectroscopy, Raman spectroscopy, Atomic absorption spectroscopy, UV/Visible spectroscopy.

Diffraction: Fundamental crystallography, Generation and detection of X-rays, Bragg's Law, X-ray diffraction at wide angle and small angles, Analysis of XRD data.

Thermal Analysis: Thermo gravimetric analysis, Differential thermal analysis, Differential scanning calorimetry.

Other analysis: Total organic carbon analyser, Particle size analysis (DLS) and Zeta Potentiometry.

Learning Resources:

Text Books:

1. S. Zhang, L. Li, Ashok Kumar, Materials Characterization Techniques, CRC Press, 2008.

Reference Books:

1. David B. Williams, C. Barry Carter, Transmission Electron Microscopy, A Textbook for Materials Science, Springer, 2009, 2nd Edition.

2. Khangaonkar P R, Penram, An Introduction to Material Characterization, Intl. Publishing (India) Pvt. Ltd, 2010.
3. B. D. Cullity and S. R. Stock, Elements of X-Ray Diffraction, Prentice Hall, 2001, 3rd Edition.

CH16034 **3-0-0 (3)**

Modelling and Simulation of Wastewater Treatment Processes

Pre-Requisites: **None**

Course Outcomes:

CO-1	Write mass and energy balances for wastewater treatment plants
CO-2	Develop mathematical models for wastewater treatment processes
CO-3	Perform uncertainty and sensitivity analyses
CO-4	Simulate the models of different units in wastewater treatment plants

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	2	1	-	1
CO-2	2	2	1	2	-	1
CO-3	2	2	3	3	-	1
CO-4	2	2	3	3	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Basic definitions in mathematical modelling and computer simulation. Problem specification, model development, modelling hydraulics, modelling oxygen transfer, model verification. Stepwise modelling framework of each unit process of an entire treatment plant.

Development of the activated sludge models: First period – empirical criteria, Second period steady-state relationships of microbial growth and organic substrate utilization, Third period complex dynamic models.

Components of a complete model of an activated sludge system: Modelling biological nutrient removal, Hydraulic configuration model, Influent wastewater characterization model, Bioreactor model, Sedimentation/clarification model. Modelling specific biochemical processes occurring in activated sludge systems.

Modelling Approaches: Anaerobic ammonium oxidation (ANNAMOX) process, Modelling of anaerobic digestion process, sequencing batch reactor, membrane bioreactor, immobilised film processes, advanced oxidation processes.

Approaches to a systematic organization of the simulation study: Data quality control including collection, verification and reconciliation. Model calibration/validation procedures, Goodness-of-fit measures, uncertainty and sensitivity analysis.

Practical model applications: Optimization of process performance, Expansion and upgradeof existing facilities, Design of new facilities, Concept of digital twin and applications in wastewater treatment plants modelling.

Learning Resources:

Text Books:

1. Jacek Makinia, Mathematical Modelling and Computer Simulation of Activated Sludge Systems,

IWA Publishers, 2010.
2. Davide Dionisi, Wastewater treatment processes: mass and heat balances, CRC Press, 2017.
3. Gustaf Olsson, BobNewell, Wastewater Treatment Systems Modelling, Diagnosis and Control, IWA Publishers, 2005.

Reference Books:

1. Mogens Henze, Willi Gujer,Takashi Mino, Mark van Loosdrecht, Activated Sludge Models - ASM1, ASM2, ASM2d and ASM3, IWA Publishers, 2000.
2. Willi Gujer, Systems Analysis for Water Technology, Springer, 2008.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103107217

CH16036 **3-0-0 (3)**

Process Intensification

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand principles of process intensification
CO-2	Design intensified processes with enhanced performance
CO-3	Develop compact heat exchangers and reactors
CO-4	Apply intensification techniques in process industries

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	-	-	2	1	3	-
CO-2	-	-	2	1	3	-
CO-3	-	-	3	1	3	-
CO-4	-	-	3	1	3	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Techniques of process intensification (PI), applications, the philosophy and opportunities of process intensification, main benefits from process intensification, process- intensifying equipment, process intensification toolbox.

Process Intensification through micro reaction technology: Effect of miniaturization on unitoperations and reactions, Implementation of micro-reaction technology, from basic propertiesto technical design rules, inherent process restrictions in miniaturized devices and their potential solutions, microfabrication of reaction and unit operation devices - wet and dry etching processes.

Scales of mixing, Flow patterns in reactors, Mixing in stirred tanks: Scale up of mixing, heat transfer, mixing in intensified equipment, chemical processing in high-gravity fields atomizer ultrasound atomization, nebulizers, high intensity inline mixers reactors static mixers, ejectors, tee mixers, impinging jets, rotor stator mixers, design principles of static mixers, applications of static mixers, higee reactors.

Combined chemical reactor heat exchangers and reactor separators: Principles of operation; applications, reactive absorption, reactive distillation, applications of RD processes, fundamentals of process modelling, reactive extraction. Case Studies: absorptionof NO_x coke gas purification. compact heat exchangers: classification of compact heat exchangers, plate heat exchangers, spiral heat exchangers, flow pattern, heat transfer and pressure drop, flat tube-and-fin heat exchangers, microchannel heat exchangers, phase-change heat transfer, selection of heat exchanger technology, feed/effluent heat exchangers,integrated heat exchangers in separation processes, design of compact heat exchanger - example.

Enhanced fields: Energy based intensifications, sono-chemistry, basics of cavitation, cavitation reactors, flow over a rotating surface, hydrodynamic cavitation applications, cavitation reactor design, nusselt-flow

model and mass transfer, the rotating electrolytic cell, microwaves, electrostatic fields, sono-crystallization, reactive separations, supercritical fluids.

Nanofluids and applications: application of PI in biochemical Engineering, biotechnology applications, fuel cells, process intensification in terms of materials point of view. Thin film reactors, application in waste water treatment of PI, photocatalytic reactors to enhance the performance using PI.

PI approaches for Energy, materials and safety: Bhopal gas tragedy case study. Sustainability-related issues in process industry, synergy.

Learning Resources:

Text Books:

1. Stankiewicz, A. and Moulijn, (Eds.), Reengineering the Chemical Process Plants, Process Intensification, Marcel Dekker, 2003.
2. David Reay, Colin Ramshaw, Adam Harvey, Process Intensification, Butterworth Heinemann, 2008.
3. Frerich Johannes Keil, Modelling of Process Intensification, Wiley VCH, 2008.

Reference Books:

1. Schmidt-Traub Henner, Gorak, Andrzej, Integrated Reaction and Separation Operations: Modelling and experimental validation,Springer, 2006, 1st Edition.
2. Hessel, V., A. Renken, J.C.Schouten and J.-I. Yoshida (eds.). Micro Process Engineering A Comprehensive Handbook, Wiley-VCH, 2009.
3. Boodhoo, K. and A. Harvey, Process Intensification for Green Chemistry: Engineering Solutions for Sustainable Chemical Processing, John Wiley & Sons Inc., 2013.

Other Suggested Readings:

1. https://ocw.tudelft.nl/courses/process-intensification/
2. https://edu.epfl.ch/coursebook/en/process-intensification-and-green-chemistry

CH16038 **3-0-0 (3)**

Electrochemical Engineering

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand thermodynamics and kinetics of electrochemical processes
CO-2	Characterize electrochemical systems using analytical instruments
CO-3	Evaluate unit operations involving electrochemical applications
CO-4	Explain the principles of electrochemical energy systems

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	3	3	1	-
CO-2	2	1	2	2	1	-
CO-3	2	1	2	3	1	-
CO-4	2	1	3	3	1	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Electrode Potentials and Thermodynamics of Cells: Basic electrochemical thermodynamics, free energy, cell emf and Nernst equation, half-cell reactions and redox potentials, reference electrodes.

Electrode Kinetics: Arrhenius equation and potential energy surfaces, transition state theory, Butler-Volmer model of electrode kinetics, current-over potentials, Tafel plots.

Electroplating: Electrochemistry fundamentals, anode-cathode reactions, Faraday's law of electrolysis, current efficiency, current density, current distribution, voltage-current relationship,over potential and over voltage, surface preparation, electrolytic metal deposition, Electrolyte, types of electroplating processes and coatings Anodizing: Aluminum anodizing, nanopores in anodized alumina, Electropolishing: Types of metals and electrolytes, characteristics of electropolished surfaces, electropolishing vs mechanical polishing, applications.

Batteries: Basic concepts, battery characteristics, classification of batteries– primary, secondary and reserve batteries, modern batteries - construction, working and applications of zinc–air, nickel-metal hydride and Li-MnO_2 batteries.

Fuel cells: Introduction, types of fuel cells - alkaline, phosphoric acid, molten carbonate, solidpolymer electrolyte and solid oxide fuel cells, construction and working of methanol-oxygen fuelcell.

Corrosion Protection: Sacrificial anodes, impressed current techniques, polarization characteristics, galvanic series, coatings.

Learning Resources:

Text Books:

1. Bard A. J., Faulkner L. R, Electrochemical Methods: Fundamentals and Applications, Wiley, 2010, 2nd Edition.
2. Fontana M. G, Corrosion Engineering, McGraw-Hill, 2008, 3rd Edition.

Reference Books:

1. Solanki C. S, Solar Photovoltaics – Fundamentals, Technologies and Applications, PHI Publishers, 2015.
2. West, Alan C., Electrochemistry and Electrochemical Engineering: An Introduction, Columbia University, 2013.
3. Hart, Lenny, Larsen and Keller, Electrochemistry and Electrochemical Engineering, 2017.

Other Suggested Readings:

1. https://nptel.ac.in/courses/113105102

CH16040 **3-0-0 (3)**

Advanced Physicochemical Treatment Technologies

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the principles of advanced physico-chemical processes
CO-2	Apply ozonation for sludge management
CO-3	Use electrochemical technologies for wastewater treatment
CO-4	Employ sonochemistry for pollutant removal

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	2	1	–	1
CO-2	2	2	1	2	–	1
CO-3	2	2	3	3	–	1
CO-4	2	2	3	3	–	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Pressurized Ozonation: Oxyozo-synthesis Sludge Management System, Oxyozo-synthesis, Wastewater Reclamation System: Ozonation and Oxygenation Process, Continuous oxygenation–ozonation, Noncontinuous oxygenation–ozonation, Formation and generation of ozone by various methods.

Requirements for ozonation equipment: Feed Gas Equipment, ozone generators and ozone contactors. In-line contactor for water treatment, Film layer purifying chamber (FLPC) contactor for water treatment, Multi compartment turbine ozone contactor. Diffuser ozone contactor properties of ozone, hyperbaric reactor vessel. Diffuser contactor for water and wastewater treatment. Properties of Ozone.

Oxygen generation systems: The traditional cryogenic air separation (CAS), pressure-swing adsorption (PSA). CAS system for oxygen production, PSA system for oxygen production, Ozonation Systems, Removal of Pollutants from Waste by Ozonation. Particle Removal Processes. Economical Aspects of Ozonation. Application of Ozone in Combined Processes.

Electrochemical Wastewater Treatment Processes: Reactors for metal recovery, rotating cylinder electrode. Fluidized bed reactor, tumbling bed electrodes. Fixed bed reactor, Design of a Reno cell. Electrode Materials, Application Areas.

Electrocoagulation: Basic concepts and theory of coagulation and flocculation with hydrolyzing metal salts. Reactions in electro-flocculation, Effect of Charge Loading, NaCl, pH Effect, Temperature, and Power Supply. Comparison of electrocoagulation and chemical coagulation.

Electro-flotation: Electrocoagulation unit with cylindrical electrodes, Effect of pH, Temperature, Alternative electrode arrangement for electro-flotation. A typical electro flotation unit design. Applications.

Electro-oxidation: Indirect EO Processes, Direct Anodic Oxidation, Typical Designs. Ultrasound assisted electrochemical treatment of wastewaters: Principles of sonochemistry. Sono-chemical destruction methods of organic pollutants. Sono-electrochemical degradation.

Sewage sludge electro-dewatering: - Sludge conditioning, Mechanical dewatering processes, Electro-dewatering process.

Learning Resources:

Text Books:

1. Lawrence K. Yung-Tse Hung, Nazih K. Shammas, Advanced Physicochemical Treatment Technologies, Humana Press, 2007.
2. Christiane Gottschalk, Judy Ann Libra, Adrian Saupe, Ozonation of Drinking Water and of Wastewater, Wiley-VCH, 2000.
3. Sillanpaa, Mika, Advanced water treatment electrochemical methods, Elsevier, 2020.

Other Suggested Readings:

1. https://onlinecourses.nptel.ac.in/noc22_ch25/preview

CH16042 **3-0-0 (3)**

Molecular Thermodynamics

Pre-Requisites: **None**

Course Outcomes:

CO-1	Determine thermodynamic properties using intermolecular forces
CO-2	Apply activity coefficient models for non-ideal systems
CO-3	Solve multiphase equilibrium problems
CO-4	Analyse molecular simulation trajectories

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	1	3	1	1	1
CO-2	3	1	3	1	1	1
CO-3	3	1	3	1	1	1
CO-4	3	2	1	3	1	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Classical Thermodynamics: First and Second laws, Property relationships, Ideal and Non- ideal gases, equation of state, Fugacity in Gas and Liquid Mixtures.

Intermolecular forces theory: Potential Energy functions, Electrostatic forces, Polarizability & Induced dipoles, Mie's potential-energy function for non-polar molecules, Structural effects, Chemical Forces.

Statistical thermodynamics: Partition function, Partition function for ideal gases, Ensembles (NVE, NVT, NPT and μVT), Equation of state, Virial equation of state for non-ideal gases.

Monte Carlo Simulations: Metropolis Algorithm, Basic Monte Carlo Algorithm, Different Trial Moves, Free Energy Calculation using Thermodynamic Integration.

Molecular dynamics simulations: Newton's Equation of Motion, Bonded and Non-bonded interactions, Sampling and averaging, Analysis of simulation using a simulation trajectory.

Application: A Case Study for Molecular System using Water Molecules.

Learning Resources:

Text Books:

1. Prausnitz J. M., Lichtenthaler R. N., Azevedo E. G., Molecular Thermodynamics of Fluid-Phase Equilibria, Prentice-Hall, 1999, 3rd Edition.
2. Sandler S. I., An Introduction to Applied Statistical Thermodynamics, Wiley, 2011, 1st Edition.
3. Donald A. McQuarrie., Statistical Mechanics, Longman Education, 2000.

Reference Books:

1. Frenkel, Daan, Berend Smit., Understanding molecular simulation: from algorithms to applications, Elsevier, 2001, Vol. 1.

2. Modell M., Reid R. C, Thermodynamics and its Applications, Prentice-Hall, 1983.
3. Tester J. W., Modell M., Thermodynamics and its Applications, Prentice-Hall, 1997, 3rd Edition.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103107208
2. https://nptel.ac.in/courses/103103162

CH16044 **3-0-0 (3)**

Statistical Design of Experiments

Pre-Requisites: **None**

Course Outcomes:

CO-1	Plan experiments for a critical comparison of outputs
CO-2	Propose hypothesis from experimental data using statistical approach
CO-3	Implement factorial and randomized sampling from experiments
CO-4	Estimate parameters by multi-dimensional optimization

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	-	-	-	-	-
CO-2	3	-	3	3	-	-
CO-3	3	-	3	3	-	-
CO-4	3	-	3	3	-	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Strategy of experimentation, basic principles, guidelines for designing experiments.

Simple Comparative Experiments: Basic statistical concepts, sampling and sampling distribution, inferences about the differences in means: Hypothesis testing, Choice of samples size, Confidence intervals, Randomized and paired comparison design.

Experiments with Single Factor: An example, The analysis of variance, Analysis of the fixedeffect model, Model adequacy checking, Practical interpretation of results, Sample computer output, Determining sample size, Discovering dispersion effect, The regression approach to theanalysis of variance, Non-parametric methods in the analysis of variance, Problems.

Design of Experiments: Introduction, Basic principles: Randomization, Replication, Blocking, Degrees of freedom, Confounding, Design resolution, Metrology considerations for industrial designed experiments, Selection of quality characteristics for industrial experiments. Parameter Estimation. Response Surface Methods: Introduction, The methods of steepest ascent, Analysis of a second-order response surface, Experimental designs for fitting response surfaces: Designs for fitting the first-order model, Designs for fitting the second-order model, Blocking in response surface designs, Computer-generated (Optimal) designs, Mixture experiments, Evolutionary operation, Robust design, Problems.

Design and Analysis: Introduction, Preliminary examination of subject of research, Screening experiments: Preliminary ranking of the factors, active screening experiment-method of randombalance, active screening experiment Plackett-Burman designs, Completely randomized block design, Latin squares, Graeco Latin Square, Youdens Squares, Basic experiment-mathematical Modelling, Statistical Analysis, Experimental optimization of research subject: Problem of optimization, Gradient optimization methods, Non-gradient methods of optimization, Simplex sum rotatable design, Canonical analysis of the response surface, Examples of complex optimizations.

Learning Resources:

Text Books:

1. Montgomery D C, Design and Analysis of Experiments, Wiley, 2013, 8th edition
2. Bradley Jones, Douglas C. Montgomery, Design of experiments: A modern approach, Wiley, 2021

Other Suggested Readings:

1. https://nptel.ac.in/courses/103106112
2. https://nptel.ac.in/courses/102106051

CH16046 **3-0-0 (3)**

Thermoset Polymer Composites

Pre-Requisites: **None**

Course Outcomes:

CO-1	Select a suitable composite production process for a given application
CO-2	Develop mathematical models for resin cure kinetics and viscosity
CO-3	Determine reinforcement fibre permeabilities
CO-4	Simulate isothermal mould filling process
CO-5	Characterize composite product for mechanical, thermal and morphological properties

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	-	1	3	-	1
CO-2	3	-	3	3	-	2
CO-3	3	-	3	3	-	2
CO-4	3	-	3	3	-	2
CO-5	3	-	3	3	-	2

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Fundamentals of Polymer Matrix Composites: Introduction of Composites, Thermoplastic and Thermoset Polymer Matrix Composites. Introduction to Resin Matrices and Reinforcement Fibres.

Composite Manufacturing Process: Introduction, Material-Manufacturing Process Property Relationship, Manufacturing of Prepeg and SMC, Molding, Resin Transfer and Vacuum Infusionmolding, Compression Molding, Filament Winding.

Resin Matrices and Reinforcement Fibres Characterization: Resin gelation and cureexotherm. Resin Cure Characterization & Modelling. Resin Cure Viscosity Characterization and Resin Rheokinetics. Fiber Porosity and Permeability. Reinforcement Mat Architecture.

Process Modelling & Simulation on Composite Processing: Continuity and Darcy's Equation, Modelling of RTM Processing, Pultrusion and Autoclave Process. General Resin Flow and Cure Model. Air Entrapment Model. Simulation Packages for Composite Processing.1-D Resin Flow Simulation.

Testing and Characterization: Characterization and Testing of Matrix Properties, Characterization and Testing of Curing Agent, Characterization and Testing of Reinforcement Properties, Characterization and Testing of Finished Product, Physical Properties, Mechanical Properties, Morphological Characterization, Fire and Toxicity, Manufacturing Defects.

Learning Resources:

Text Books:

1. Sanjay Majumdar, Composites Manufacturing Materials, Product, and Process Engineering, CRC press, 2002.
2. P.K. Mallick, Fiber-reinforced Composites: materials, manufacturing, and Design, CRC press,

2007, 3rd Edition.

3. Suresh G.A, Sozer E.M, Process Modelling in Composite Manufacturing, CRCpress, 2nd Edition.

CH16048 **3-0-0 (3)**

Molecular Simulations

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the concepts of ensembles and interatomic potentials
CO-2	Simulate different ensembles using Monte Carlo and molecular dynamics techniques
CO-3	Compute thermodynamic properties
CO-4	Simulate a real life problem using molecular dynamics and Monte Carlo methods

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	–	2	3	–	2
CO-2	3	–	2	3	–	2
CO-3	3	–	2	3	–	2
CO-4	3	–	2	3	–	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Thermodynamics and statistical mechanics: Classical thermodynamics; Statistical thermodynamics; Ensembles; Ergodicity.

Monte Carlo simulations: Monte Carlo method; a basic Monte Carlo method; Trial Moves.

Molecular dynamics simulations: Molecular dynamics initialization; solving equations of motion.

Properties computation: Static properties; Dynamical properties.

Ensemble simulations: Monte Carlo simulations in various ensembles, Molecular dynamics simulation in various ensembles.

Learning Resources:

Text Books:

1. Daan Frenkel, Berend Smit, Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, 2023, 3rd Edition.
2. M. P. Allen, D. J. Tildesley, Computer Simulations of Liquids, Oxford University Press, 2017, 2nd Edition.

Reference Books:

1. Andrew Leach, Molecular Modelling: Principles and Applications, Prentice Hall, 2001, 2nd Edition.
2. D.C. Rapapport, The art of Molecular Dynamics Simulation, Cambridge university press, 2004, 2nd Edition.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103103036

CH16050 **3-0-0 (3)**

Heat Integration and Process Scheduling

Pre-Requisites: **None**

Course Outcomes:

CO-1	Identify the objectives of heat integration and process scheduling
CO-2	Apply the concepts of pinch technology and retrofitting
CO-3	Develop models for batch process scheduling
CO-4	Analyze heat exchanger networks and process scheduling models

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	1	1	1	1
CO-2	2	1	3	3	1	1
CO-3	2	1	3	3	1	1
CO-4	2	3	3	3	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Heat Integration:

Introduction: Heat integration fundamentals; History and industrial experience; Why does pinch analysis work; The concept of process synthesis; The role of thermodynamics in process design.

Key concepts of Pinch analysis: Heat recovery and heat exchange; The pinch and its significance; Heat exchanger network design; Choosing ΔT_{min}; Methodology of pinch analysis.

Data extraction and energy targeting: Data extraction; Case study: Organics distillation plant, Energy targeting, Multiple utilities, Targeting heat exchanger units, Area and shells, Super targeting, Targeting organics distillation plant case study.

HEN Design Utilities: Heat exchange equipment; Stream splitting and cyclic matching; Network relaxation; More complex designs; Multiple pinches and near pinches; Retrofit design.

Process Scheduling:

Short-Term Scheduling: Effective technique for scheduling of multipurpose and multi product batch plants; Different storage policies for intermediate and final products; Evolution of multiple time grid models in batch process scheduling; Short-term scheduling of multipurpose plants; Planning and scheduling in chemical and biopharmaceutical industry.

Heat integration in multipurpose batch plants: Direct and indirect heat integration; Simultaneous optimization of energy and water use in multipurpose batch plants.

Design and Synthesis: Design and synthesis of multipurpose batch plants; Process synthesis approaches for enhancing sustainability of batch process plants; Scheduling and design of multipurpose batch facilities.

Learning Resources:

Text Books:

1. Ian C Kemp, Pinch Analysis and Process Integration, Elsevier Publication, 2007, 2nd Edition.
2. Thokozani Majozi, Esmael Reshid Seid, Jui-Yuan Lee, Synthesis, Design, and Resource Optimization in Batch Chemical Plants, CRC Press, 2015.

Reference Books:

1. Thokozani Majozi, Batch Chemical Process Integration - Analysis, Synthesis and Optimization, Springer, 2010.
2. Mohmoud Bahy Noureddin, Pinch Technology and Beyond Pinch, New Vistas on Energy Efficiency Optimization, Booktopia, 2011.
3. Gintaras V. Reklaitis, Aydin K. Sunol, David W. T. Rippin, Oner Hortacsu, Batch Processing Systems Engineering, Springer, 1996.
4. Mariano Martin, Introduction to Software for Chemical Engineers, CRC Press, 2015.

CH16052 **3-0-0 (3)**

Statistical Thermodynamics

Pre-Requisites: **None**

Course Outcomes:

CO-1	Identify the molecular level properties influencing the macroscopic thermodynamic properties
CO-2	Develop models to estimate thermodynamic properties of real gases, liquids and solids
CO-3	Design molecular level architecture to enhance macroscopic properties
CO-4	Estimate macroscopic properties based on molecular level interactions

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	-	3	1	-	1
CO-2	2	-	3	1	-	1
CO-3	2	-	3	1	-	1
CO-4	2	-	3	1	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Basics of Statistical Thermodynamics: The Statistical Foundation of Classical Thermodynamics, Classification Scheme for Statistical Thermodynamics, Importance of Statistical Thermodynamics.

Ensembles: Ensembles and Postulates, Canonical Ensemble, Canonical Ensemble and Thermodynamics, Grand Canonical Ensemble, Micro Canonical Ensemble, Thermodynamic Equivalence of Ensembles.

Evaluation of Probabilities: Probability- Definitions and Basic Concepts, Permutations and Combinations, Distribution Functions: Discrete and Continuous, Binomial Distribution, Poisson Distribution, Gaussian Distribution, Combinatorial Analysis for Statistical Thermodynamics.

Criteria for Equilibrium: Equilibrium Principles, States of Equilibrium: Neutral, Metastable, and Unstable equilibrium, Maximizing Multiplicity.

Model for Mono-atomic and Polyatomic Ideal Gases: Energy Levels and Ensembles, Partition Function, Thermodynamic Functions for Mono-atomic Ideal Gases, Internal Degrees of Freedom, Independence of Degrees of Freedom, Potential Energy Surface, Vibration, Rotation, Thermodynamic Functions for Poly-atomic Ideal Gases, Hindered Internal Rotation in Ethane, Hindered Translation on a Surface, Fluctuation Theory. Einstein's and Debye's Model of the Solid, Simple Liquids, Phase Equilibrium, Models for Multi Component Systems: Ideal Lattice Gas, Lattice Gas with Interactions, Solutions (Bragg- William Model and Regular Solutions, Quasi-Chemical Model).

Learning Resources:

Text Books:

1. Terrell L. Hill, An Introduction to Statistical Thermodynamics, Courier Corporation, 2012.
2. Donald A. McQuarrie, Statistical Mechanics, Viva Books Pvt. Ltd., 2018.
3. Normand M. Laurendeau, Statistical Thermodynamics: Fundamentals and Applications, Cambridge University Press, 2005.

Reference Books:

1. Leonard K. Nash, Elements of Statistical Thermodynamics, Dover Publications, 2006, 2nd Edition.
2. Stanley I. Sandler, An Introduction to Applied Statistical Thermodynamics, John Wiley &Sons, 2015, 1st Edition.
3. Herbert B. Callen, Thermodynamics and Introduction to Thermo-statistics, Wiley, 1985, 2nd Edition.

Other Suggested Readings:

1. https://nptel.ac.in/courses/103103355
2. https://nptel.ac.in/courses/115106126

CH16054 **3-0-0 (3)**

Computational Catalysis

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the basic concepts & methods in computational catalysis
CO-2	Acquire basic knowledge about Density Functional theory (DFT)
CO-3	Describe different computational methods of catalysts in macroscopic level size
CO-4	Apply computational methods to find different properties of the catalysts

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	-	1	1	-	2
CO-2	3	-	1	3	-	2
CO-3	3	-	1	3	-	3
CO-4	3	-	1	3	-	3

1 - Slightly; **2 - Moderately;** **3-Substantially**

Syllabus:

Introduction: Behavior of materials, Design of catalysts electronic level to industrial application, Methods and applications of computational catalysis**,** Sabatier principle, Volcano plots, BrΦnsted Evans-Polanyi (BEP) scaling relations, Industrial requirements for efficient catalysts, Tools for computational catalysis, Limitations.

Density Functional Theory (DFT): The Schrödinger Equation, Hohenberg - Kohn (HK) theorems, Kohn-Sham (KS) equations, Wave Functions to Electron Density, Exchange-Correlation Functional, Pseudopotentials (PP), Ground state properties, Electron density approximations, minimizing of total energy, Self-consistent filed (SCF), Gaussian functions (Cluster models) & Periodic functions (crystal models), Basis set, Algorithm of DFT, Practical examples, Challenges in DFT calculations.

Molecular dynamics: Ab Initio molecular dynamics- Born-Oppenheimer molecular dynamics (BOMD), Car-Parrinello molecular dynamics (CPMD), Error estimation in CPMD, Classical molecular dynamics-Force Field Methods, Making reactive Force Field (ReaxFF), Transferability &Training of ReaxFF, Difficulties in ReaxFF.

Statistical methods: Rare event dynamics, mapping to lattice, mean filled approximation, Kinetic Monte Carlo (KMC) simulations, CO oxidation with Pt surface.

Properties: Adsorption of small molecules on solid surfaces and clusters, Solvation model environment, Vibrational properties (Infrared spectroscopy), Reaction mechanism (energy barriers), interaction between reacting species in a reaction.

Learning Resources:

Text Books:

1. Rutger A. van Santen, Philippe Sautet, Computational Methods in Catalysis and Materials Science:

An Introduction for Scientists and Engineers, Wiley-VCH, 2009.
2. Asthagiri A, Janik MJ, editors. Computational catalysis, Royal Society of Chemistry, 2023, 2nd Edition.

Reference Books:

1. F. Giustino, Materials Modelling using Density Functional Theory, Oxford University Press, 2014, 1st Edition.
2. J. G. Lee, Computational materials science: an introduction, CRC press, 2011, 2nd Edition.

CH16060 **3-0-0 (3)**

Advanced Process Control

Pre-Requisites: **None**

Course Outcomes:

CO-1	Identify controlled and manipulated variables
CO-2	Design regulatory control schemes for a given process
CO-3	Analyse the multivariable process control schemes
CO-4	Evaluate linear and nonlinear model predictive control strategies

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	1	3	3	–	2
CO-2	3	1	3	3	–	2
CO-3	3	1	3	3	–	2
CO-4	3	1	3	3	–	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Hierarchy of control layers, review of basics, system linearization, state space and transfer function models.

Advanced regulatory control schemes: Cascade control, feed-forward control, ratio control, split-range control, time delay compensator, and inverse response compensator.

Multivariable control: Challenges, Control pairing; Interactions in closed-loop systems; Relative Gain Array (RGA) and variants. Centralized, decentralized, decoupled control schemes.

Model Predictive Control (MPC): MPC control formulation: simple unconstrained optimal control formulation, general characteristics of MPC formulation, translation of MPC problem into quadratic programming optimization problem, Practical MPC implementation considerations: empirical model development, usage of design/tuning parameters, design of MPC control for typical systems.

Extensions of MPC: Theory: Economic MPC, Nonlinear Model Predictive Control (NMPC), Robust MPC, Data-driven MPC.

Learning Resources:

Text Books:

1. Seborg, D. E., Edgar, T. F., Millechamp, D. A., Doyle III, F. J., Process Dynamics and Control, Wiley, 2014, 3rd Edition.
2. Raghunathan Rengaswamy, Babji Srinivasan, Nirav Pravinbhai Bhatt, Process Control Fundamentals: Analysis, Design, Assessment, and Diagnosis, CRC Press, 2020.
3. Liuping Wang, Model Predictive Control System Design and Implementation using MATLAB, Springer, 2009.

Reference Books:

1. Francesco Borrelli, Alberto Bemporad, Manfred Morari, Predictive Control for Linear and Hybrid Systems, Cambridge University Press, 2017.
2. Jean-Pierre Corriou, Process Control: Theory and Applications, Springer, 2018, 2nd Edition.
3. B. Roffel, B. Betlem, Process Dynamics and Control, Wiley, 2006.
4. Cecil L. Smith, Advanced Process Control, Wiley, 2010.
5. Surekha Bhanot, Process Control: Principles and Applications, Oxford, 2008.

Other Suggested Readings:

1. https://onlinecourses.nptel.ac.in/noc21_ge01/preview

ME16062 **3-0-0 (3)**

Thermal Energy Storage

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the principles, concepts, and operation of thermal energy storage systems
CO-2	Select the suitable energy storage materials
CO-3	Design thermal energy storage systems
CO-4	Evaluate the performance of thermal energy storage systems for different applications

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	1	1	2	1	1
CO-2	1	1	1	2	1	1
CO-3	1	1	2	3	1	1
CO-4	1	1	2	3	1	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Classification of Energy Resources, Energy Scenario in the World and India, Need for Energy Efficiency, Energy Conservation and Management.

Introduction to Thermal Energy Storage Systems: Introduction, Thermodynamics of Energy Storage, System Types, Environmental Impact.

Sensible Heat Storage Systems: Introduction, Types, Principles of Sensible Heat Storage Systems, Limitations, Advantages and Future Trend.

Latent Heat Storage Systems (Phase Change Materials): Introduction, Types, Selection Criteria, Thermophysical Properties, Thermal Stability, Corrosion, Phase Segregation, Sub Cooling, Applications.

Microencapsulation and Nanoencapsulation of Phase Change Materials: Introduction, Microencapsulation and Nanoencapsulation of Phase Change Materials, Methods, Shape Stabilized Phase Change Materials, Applications.

Design of Latent Heat Storage System: Introduction, Requirements and Considerations for the Design, Design Methodologies, Applications of Latent Heat Storage Systems Incorporating PCMS, Future Trends.

Modelling of Heat Transfer in Phase Change Materials (PCMS): Introduction, Inherent Physical Phenomena in Phase Change Materials, Modelling Methods and Approaches for the Simulation of Heat Transfer in PCMS for Thermal Energy Storage, Examples of Modelling Applications, Future Trends.

Phase Change Materials for Energy Conservation in Buildings: Introduction, Integration of PCMS into Building Envelop, PCM Containment, Measurement of Thermal Properties of PCM Integrated in Buildings, Experimental and Numerical Studies.

Thermochemical Heat Storage: Introduction, Phenomena and Principles, Thermochemical Energy Storage Systems, Applications, Remarks.

Thermal Energy Storage Systems Applications: Introduction, Solar Air Heating, Solar WaterHeating, District Heating, Heat to Waste, Cogeneration and Trigeneration Systems, Concentrated Solar Power, Cooling.

Learning Resources:

Text Books:

1. Kalaiselvam, S., Parameshwaran, R., Thermal Energy Storage Technologies for Sustainability Systems Design, Assessment and Applications, Elsevier, 2014.
2. Luisa F.Cabeza, Advances in Thermal Energy Storage Systems - Methods and Applications, Elsevier, 2015.

Reference Books:

1. Ibrahim Dinçer, Marc A. Rosen, Thermal Energy Storage: Systems and Applications, John Wiley & Sons Ltd., 2010.

CH26002 **3-0-0 (3)**

Electrochemical Energy Storage Systems

Pre-Requisites: **None**

Course Outcomes:

CO-1	Explain fundamental electrochemical principles such as redox reactions, cell potentials, and ionic conductivity of electrolytes
CO-2	Apply electrochemical techniques like cyclic voltammetry and galvanostatic charge-discharge to characterize electrochemical systems
CO-3	Analyze various battery technologies and their components, focusing on performance and key characteristics
CO-4	Describe the design and functionality of flow batteries, including the roles of electrodes, electrolytes, membranes, and stack design
CO-5	Evaluate the principles, materials, and applications of supercapacitors, comparing them with batteries and identifying challenges and future directions
CO-6	Analyze various recycling processes for energy storage systems and their impact on sustainability and environmental challenges

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	2	-	1	-	1
CO-2	1	2	-	1	-	1
CO-3	1	2	-	2	-	1
CO-4	3	3	-	1	-	1
CO-5	1	3	-	1	-	1
CO-6	1	3	-	2	-	1

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Battery Fundamentals and Technologies: Electrochemical energy storage mechanisms. cell vs. battery. History of battery development. Battery Classification: Primary and secondary batteries; Based on electrode materials and electrolytes (aqueous vs. non-aqueous).

Existing Battery Systems: Basic operation and key characteristics (Lead-Acid, Nickel Cadmium, Nickel Hydrogen, Nickel Metal Hydride). Lead acid batteries: Effect of Temperature- Peukert's Law, Discharge Rate, Sulfation, Overcharging, Plate Thickness; Nickel cadmium: components, advantages and limitations.

Lithium-Ion Batteries: Classification: Based on cathode and anode materials (LFP, LCO). Working Principle: Charge/discharge cycles, role of the electrolyte. Critical Components and Materials: Anode Materials: Graphite, silicon, lithium titanate; Cathode Materials: Layered oxides, spinel oxides, olivine phosphates. Electrolytes: Organic solvents with lithium salts, ionic conductivity, safety. Separators: Microporous polymer membranes. Advantages and Limitations: Capacity, cycling stability, safety.

Advanced Battery Technologies: Lithium-Air Batteries: Ultra-high energy density potential, working principle, challenges (electrode stability, electrolyte decomposition). **Sodium-Ion Batteries:** History, working mechanism, components and materials (anodes: hard carbon, sodium titanate; cathodes: layered oxides, polyanionic compounds), advantages and limitations. **Aluminum-Ion Batteries:** Introduction, historical development, rechargeable types (chloroaluminate, aluminum-sulfur), specific requirements for electrolytes, challenges, and future prospects. **Dual-Ion Batteries**: Working mechanism, cathode and anode materials, advantages and limitations.

Flow Batteries: Concept and Working Principle. Electrolytes: Different redox couples and performance properties; Electrodes: Porous carbon materials; Membranes and Stack Design: Flow field design, materials selection.

Supercapacitors: Introduction and Comparison with Batteries: Basic principles (electric charge, electric field, potential, capacitance), charging/discharging, energy storage mechanisms. Materials for Supercapacitors: Electrolytes: Aqueous, organic, ionic liquids. Energy Storage Mechanisms: Electrostatic vs. pseudocapacitive. Electrode materials: Carbon materials (activated carbon, CNTs, graphene), metal oxides/sulfides, conducting polymers.

Recycling Processes: Recycling Methods: Hydrometallurgy, pyrometallurgy, chemical, biological, direct recycling. Future Prospects: Innovations and sustainability in recycling technologies.

Learning Resources:

Text Books:

1. Allen J. Bard, Larry R. Faulkner, Electrochemical Methods: Fundamentals and Applications, Wiley, 2000, 2nd Edition.
2. Beard, K.W., Linden's handbook of batteries. McGraw Hill Education, 2019.
3. Brian E. Conway, Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications, Volume: 1, Springer, 1999.

Reference Books:

1. Vladimir S. Bagotsky, Alexander M. Skundin, Yurij M. Volfkovich, Electrochemical Power Sources: Batteries, Fuel Cells, and Supercapacitors, Wiley, 2015.
2. Aiping Yu, Victor Chabot, Jiujun Zhang, Electrochemical Supercapacitors for Energy Storage and Delivery: Fundamentals and Applications, CRC Press, 2017, 1st Edition.
3. François Béguin, Elżbieta Frąckowiak, Supercapacitors: Materials, Systems, and Applications, Wiley, 2013.
4. Warner, J. T., The Handbook of Lithium-Ion Battery Pack Design: Chemistry, Components, Types and Terminology, Elsevier, 2015.