

**R-23**

**M.Tech.Program Regulations**

**Scheme of Instruction & Syllabus**

(Effective from the Batch Admitted in 2020-2021)



**DEPARTMENT OF CHEMICAL ENGINEERING**

**V UNIVERSITY COLLEGE OF ENGINEERING**

**TIRUPATI- 517502**

**CH11C****ADVANCED TRANSPORT PHENOMENA**

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

**Objectives:**

1. To familiarize the student with basic concepts of transport phenomena and brief review of mathematics.
2. To enable students to understand the equations of change for isothermal flow and for non-isothermal flow.
3. To introduce the details of equations of change for multicomponent systems.
4. To give them insight into properties of two-dimensional flows and aspects of dimensional analysis

**Unit-1:** 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, Turbulent Flow in Jets.

**Unit-2:** 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, Use of the Equations of Change to Solve Steady-State Problems, Dimensional Analysis of the Equations of Change for Non-Isothermal Systems.

**Unit-3:** 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, Steady Heat Conduction in Laminar, Incompressible Flow. 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.

**Unit-4:** Macroscopic Balances For Non-Isothermal Systems: Macroscopic Energy Balance, Macroscopic Mechanical Energy Balance, Use Of The Macroscopic Balances To Solve Steady State 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, Steady-State Transport in Binary Boundary Layers, Concentration Distributions in Turbulent Flow -

Concentration Fluctuations and the Time-Smoothed Concentration, Time-Smoothing of the Equation of Continuity of A, Semi-Empirical Expressions for the Turbulent Mass Flux, Enhancement of Mass Transfer by a First-Order Reaction in Turbulent Flow.

**Unit -5:** 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.

### References

- 1) Thomson W.J., Transport Phenomena, Pearson Education, Asia, 2001.
- 2) Geankopolis C.J., Transport Processes and Unit Operations, 4th Ed., Prentice Hall (India) Pvt. Ltd., New Delhi. 2004.
- 3) Bird R.B., Stewart W.E. and Lightfoot E.N., Transport Phenomena, Revised 2nd Edition, John Wiley & Sons, 2007.

**Outcomes:** At the end of the course, the student will be able to:

1. Understand the mechanism of momentum, heat and mass transport for steady and unsteady flow.
2. Perform momentum, energy and mass balances for a given system at macroscopic and microscopic scale.
3. Solve the governing equations to obtain velocity, temperature and concentration profiles.
4. Model the momentum, heat and mass transport under turbulent conditions.
5. Develop analogies among momentum, energy and mass transport.

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

## CH12C

## SEPARATION PROCESSES

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives:

- 1) Understand the classification of separation processes
- 2) To learn the fundamental concepts of rate governed processes
- 3) To impart the basic concepts of multistage separation processes
- 4) Understand the design of distillation column using different methods
- 5) Understand the energy requirements of different separation processes

## UNIT I

**Use and Characteristics of Separation Processes** – Importance and variety of Separations – Characteristics of separation Processes- Inherent separation factors for equilibrium and rate Governed Processes

**Simple equilibrium processes:** Equilibrium calculations- Checking phase conditions for a mixture- Analysis of simple equilibrium separation processes for binary and multicomponent systems - Computational and Graphical Approaches.

## Unit II

**Additional Factors Influencing Product Purities** – Incomplete Mechanical Separation of Product Phases – Flow Configuration and Mixing Effects – Batch Operations – Methods of Regeneration – Mass and Heat Transfer Limitations – Stage Efficiencies

**Multistage Separation Processes:** Increasing product purity - Reducing consumption of separating agent - co-current, crosscurrent and countercurrent flow - Other separation processes - Fixed bed processes.

## Unit-III:

**Binary Multistage Separations - Distillation:** Binary Systems - Equilibrium stages and McCabe-Thiele Diagram - design and other problems – Multistage batch distillation- Straight operating lines and curved operating lines.

## UNIT IV

**Patterns of Change:** Binary and Multicomponent multistage separations

**Group Methods** - Linear stage-exit relationships and constant flow rates - nonlinear stage – Exit Relationships and varying flow rates.

**Capacity of contacting devices:** factors limiting capacity and factors influencing efficiency.

## UNIT V

**Energy Requirements of separation processes:**

Thermodynamic efficiency - single stage and multistage separation processes - reduction of energy consumption.

**Selection of Separation processes:** Factors influencing the choice of separation Process - solvent extraction and Illustrative examples

**TEXTBOOKS:**

1. Separation Processes - C. Judson King, McGraw-Hill, 1982

**REFERENCE BOOKS**

1. Separation Process Principles - J.D. Seader and E.J. Henley, John Wiley, 1998.
2. Mass Transfer Operation - R.E. Treybal, 3<sup>rd</sup> edition - McGraw-Hill 1980
3. Transport Processes and Unit Operations - Geankoplis C.J. 4<sup>th</sup> ed - PHIPvt. Ltd

**Course Outcomes:** Student will be able to

- 1) Apply the concepts of diffusion mass transfer, mass transfer coefficients, convective mass transfer, inter-phase mass transfer, equipment for gas-liquid operations
- 2) Suggest and design equipment for various mass transfer operations
- 3) Study of the stage wise mass transfer operations, principles of various stage wise contact processes like distillation
- 4) Student will be able to select a separation process for a particular system.
- 5) Able to understand the energy requirements of separation processes

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

## CH13C

## CHEMICAL REACTOR THEORY

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Course Educational Objectives:

- 1) The emphasis of this course is on the fundamentals of chemical reaction kinetics and chemical reactor operation.
- 2) The overall goal of this course is to develop a critical approach toward understanding complex reaction systems and elucidating chemical reactor design.
- 3) Integrate concepts from science & engineering to constitute a basis for the design of chemical reactor, a key element in the design of chemical process.
- 4) Provide a foundation on Non-ideal reactors and RTD
- 5) Impart knowledge about heterogeneous catalytic reactors

### UNIT I

**Isothermal Reactor design:** Design structure for isothermal reactors - Scale-up of liquid phase batch reactor data to the design of a CSTR - Tubular reactors - Pressure drop in Reactors - Reversible reactions - unsteady state operation of reactors - Simultaneous reaction and Separation.

### UNIT-II

**Analysis of Non ideal Reactors** - RTD - Measurement and characteristics of RTD - RTD in ideal reactors - Reactor modeling with the RTD - Zero and One parameter models - Two-Parameter model - Modeling real reactors with combinations of ideal reactors - Testing a model and determining its parameters - Other models of non ideal reactors using CSTRs and PFRs

### UNIT-III

**External diffusion Effect on Heterogeneous Reactions** - Binary diffusion - External resistance to mass transfer - the shrinking core model.

**Diffusion and reaction in Porous Catalyst** - Diffusion and reaction in spherical pellets - Internal Effectiveness factor - Falsified Kinetics - Overall effectiveness factor - Estimation of diffusion and reaction limited regimes - Mass transfer and reaction in a packed bed

### UNIT-IV

#### Internal Transport Processes - Reaction and Diffusion in porous catalysts:

Intra pellet mass transfer and intra pellet heat transfer, Mass transfer with reaction, Mass and Heat transfer with reaction, effect of internal transport on selectivity and poisoning.

### UNIT-V

**Design of heterogeneous Catalytic Reactors:** Fixed bed reactors and isothermal and adiabatic fixed-bed reactors, non isothermal, non adiabatic fixed bed reactors, Two phase model, Fluidized-Bed reactors, Operating characteristics of FBRs. Mass Transfer in Fluidized Beds: Gas-Solid Mass Transfer, Mass Transfer between the Fluidized-Bed Phases, Reaction in Fluidized Bed. Trickle bed reactor Models, Slurry reactor models.

## TextBooks

1. J.M.Smith“ChemicalEngineeringKinetics”3<sup>rd</sup>ED.,McGrawHill,NewYork1980
2. FoglerH.S.,ElementsofChemicalReactionEng.”,3<sup>rd</sup>Ed.,PrenticeHall,1999
3. Levenspiel,O.,“ChemicalReactionEng.”JohnWiley&Sons1972.

## CourseOutcomes:Student willbeableto

- 1) learntheimportanceofRTDandNon-idealflowinreactingvessels.
- 2) Calculate the conversions based on segregated flow model, dispersion model and tanks-in-series models.
- 3) Understandthediffusionandreactioninaporouscatalyst.
- 4) Learnthe factorsinfluencing catalystdecay,therole ofpore diffusion on catalystactivity rate.
- 5) Understandthedesignofheterogeneouscatalyticreactors.

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

## **CH16L      COMPUTATIONAL TECHNIQUES LABORATORY**

Instruction, hours/week: 4

Credits: 2

Assessment: 40+60

### **Objectives:**

1. To learn Numerical methods for interpolation, extrapolation, graphical differentiation and integration, curve fitting.... Process Modeling and Simulation of Chemical operations and processes.
2. To implement the above on MATLAB

### **List of experiments:**

- |   |   |
|---|---|
| 1. Euler Method                         | 2. Runge Kutta 4 <sup>th</sup> Order Method |
| 3. Jacobi Iteration Method              | 4. Gauss-Siedel Iteration Method            |
| 5. Lagrange's Iteration Method          | 6. Newton Forward Interpolation Method      |
| 7. Newton Backward Interpolation Method | 8. Bisection Method                         |
| 9. Newton Raphson Method                | 10. Regula Falsi Method                     |

### **Outcomes:** At the end of the course, the student will be able to:

1. Use numerical methods for various manipulations and be capable of implementing them on a computing system.

## **CH17L      ADVANCED CHEMICAL ENGINEERING LABORATORY**

Instruction, hours/week: 4

Credits: 2

Assessment: 40+60



## **PGPC01            Research methodology and IPR**

Instruction Hours/Week: 3

Credits: 3

Sessional Marks            : 40

End Semester Examination Marks: 60

### **DESCRIPTION OF THE COURSE:**

This subject gives how to proceed systematically for research, present research findings. This course consists of basics of research methods, paper writing, patenting methods and requirements..

### **COURSE EDUCATIONAL OBJECTIVES (CEOs):**

1. To understand the importance of research objectives and procedures
2. To know the procedures of data collection and report writing of research.
3. To have the knowledge of filing and obtaining a patent on research findings.

#### **UNIT I**

Meaning, Objective and Motivation in Research: Types of Research, Research Approaches, Research Process, Validity and Reliability in Research, Research Design: Features of Good Design, Types of Research Design, Basic Principles of Experimental Design

#### **UNIT II**

Sampling Design: Steps in Sampling Design, Characteristics of a Good Sample Design, Random Samples and Random Sampling Design Measurement and Scaling Techniques: Errors in Measurement, , Scaling and Scale Construction techniques, Forecasting Techniques, Time Series Analysis, Interpolation and Extrapolation

#### **UNIT III**

Methods of Data Collection: Primary Data, Questionnaire and Interviews, Collection of Secondary Data, Cases and Schedules. Professional Attitude and Goals, Concept of Excellence, Ethics in Science and Engineering, Correlation and Regression Analysis, Method of Least Squares, Regression Vs. Correlation, Correlation Vs. Determination.

#### **UNIT IV**

Interpretation of Data and Report Writing, Layout of a Research Paper, Techniques of Interpretation. Making Scientific Presentation at Conferences and Popular Lectures to Semi Technical Audience, Participating in Public Debates on Scientific Issues

#### **UNIT V**

Nature of Intellectual property rights, Patents, designs, trademarks and copyrights, History of patenting, process of patenting, patent development, international cooperation on IPR, procedure of granting patent, patent rights, licensing and transferring technology, Geographical Indications, IPR in biological and systems and software.

**Text/Reference Books:**

1. Research Methodology: Methods And Techniques - C.R. Kothari, 2nd Edition, New Age International Publishers.
2. Statistical Methods - SP. Gupta. S. Chand & Sons, New Delhi.
3. Intellectual Property - the law of trademarks, copyrights, Patents, and trade secrets - Deborah E. Bouchoux, Esq. Georgetown University, Fourth edition

**Course Outcomes (COs):**

1. Able to know research importance and requirements and procedure
2. Able to apply sampling techniques for analysis and forecasting.
3. Able to use methods for data collection and analyze the data using different mathematical techniques.
4. Able to write report on research done and present the research findings in systematic manner.
5. Able to have the knowledge to file and obtain patent on research finding.

## CH14C

## PROCESS DESIGN AND SYNTHESIS

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives:

1. To understand the systematic approaches for the development of conceptual chemical process designs
2. To learn the advances in problem formulation and software capabilities which offer the promise of a new generation of practical process synthesis techniques based directly on structural optimization.
3. Learning chemical process synthesis, analysis, and optimization principles
4. Product design and development procedure and Process life cycle assessment.

### Unit I: Introduction

Introduction to fundamental concepts and principles of process synthesis and design and use of flowsheet simulator to assist process design. Process Flowsheet Models: An Introduction to Design, Chemical process synthesis, analysis and optimization. Introduction to commercial process design software such as HYSYS, Aspen plus etc., Chemical Process (reactor, heat exchanger, distillation etc) analysis using commercial software

### Unit II: Product design and developments

Process engineering economics and project evaluation Life Cycle Assessments of process: From design to product development, Engineering Economic Analysis of Chemical Processes, Project costing and performance analysis, Environmental concerns, Green engineering, Engineering ethics, Health and safety.

### Unit III: Reactor Networks

Geometry of mixing and basic reactor types, The Attainable Region (AR) approach, AR in higher dimensions & for other processes, Reactive Separation processes, Fundamental behavior and problems, Separation through reactions. Reactive Residue Curve Maps

### Unit IV: Synthesis of Separation Trains

Criteria for selection of separation methods, selection of equipment: Absorption, Liquid-liquid extraction Membrane separation, adsorption, leaching, drying, crystallization, Ideal distillation - Column and sequence fundamentals, Sharp splits & sequencing Phase diagrams for 2, 3 and 4 components, Feasibility and vapor flow rates for single columns, Residue curve basics, Non-ideal Distillation-Azeotropic systems; detecting binary azeotropes, Residue curve maps for azeotropic systems, Topological analysis, Feasibility for single azeotropic columns, Binary VLE and pressure-swing separation, Non-ideal distillation synthesis. Equipment sequencing: VLE + VLLE, Detailed Residue Curve Maps, Residue curve maps: Interior structure

## Unit V: Heat Exchanger Network Synthesis

Minimum heating and cooling requirements, Minimum Energy Heat Exchanger Network, Loops and Paths, Reducing Number of Exchangers, HENS basics & graphics, The pinch point approach, Stream Splitting, Performance targets, trade-off & utilities, Heat & power integration, HENS as mathematical programming

### References

1. Douglas, J. "Conceptual Design of Chemical Processes", New York, NY: McGraw-Hill Science/Engineering/Math, 1988. ISBN: 0070177627.
2. Seider, W.D., J.D. Seader, and D.R. Lewin. "Product and Process Design Principles: Synthesis, Analysis, and Evaluation", 2nd ed. New York, NY: Wiley, 2004. ISBN: 0471216631.
3. Richard Turton, Richard C. Bailie, Wallace B. Whiting, Joseph A. Shaeiwitz., "Analysis, Synthesis, and Design of Chemical Processes", 2nd Edition, 2002, Prentice Hall ISBN-10: 0-13-064792-6
4. Biegler L.T., Grossmann I.E. and Westerberg A.W., "Systematic Methods of Chemical Process Design", Prentice Hall, 1997.

**Outcomes:** At the end of the course, the student will be able to

1. Analyze alternative processes and equipment
2. Synthesize a chemical process flowsheet that would approximate the real process
3. Design best process flowsheet for a given product
4. Perform economic analysis related to process design and evaluate project profitability
5. Heat Exchanger Network Synthesis

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

## CH14C

## FLUIDIZATION ENGINEERING

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives

1. To study the phenomenon of fluidization with industrial processing objective
2. To study the various regimes of fluidization and their mapping.
3. To study the design of equipments based on fluidization technique

### Unit I: Introduction to fluidization and applications

Phenomenon of fluidization, behavior of fluidized bed, contacting modes, advantages and disadvantages of fluidization, fluidization quality, selection of contacting mode, Beds for Industrial applications, coal gasification, synthesis reactions, physical operations, cracking of hydrocarbons

### Unit II: Mapping of fluidization regimes

Characterization of particles, mechanics of flow around single particles, minimum fluidization velocity, pressure drop versus velocity diagram, The Geldart classification of solids, fluidization with carryover of particles, terminal velocity of particles, distributor types, gas entry region of bed, pressure drop requirements, design of gas distributor, power consumption

### Unit III: Bubbling fluidized beds

Davidson model for bubble in a fluidized bed, and its implications, the wake region and movement of solids at bubbles, coalescence and splitting of bubbles, bubble formation above a distributor, slug flow, Turbulent and fast fluidization - mechanics, flow regimes and design equations, Emulsion movement, estimation of bed properties, bubble rise velocity, scale up aspects, flow models, two phase model, K-L model

### Unit IV: Solids movement and Gas dispersion

Vertical and horizontal movement of solids, Dispersion model, large solids in beds of smaller particles, staging of fluidized beds

Gas dispersion in beds, gas interchange between bubble and emulsion, estimation of gas interchange coefficient, Heat and mass transfer in fluidized systems, Mixing in fluidized systems - measurements and models.

### Unit V: Fluidized bed reactors

Entrainment and elutriation, Freeboard behavior, gas outlet, entrainment from tall vessel, freeboard entrainment model, high velocity fluidization, pressure drop in turbulent and fast fluidization, Slugging, Spouted beds, Circulating Fluidized Beds.

Mathematical model of a homogeneous fluidized bed, Design of catalytic reactors, pilot plant reactors, information for design, bench scale reactors, design decisions, deactivating catalysts, Design of non-catalytic reactors, kinetic models for conversion of solids, models for shrinking particles, conversion of solids of unchanging size]

## References

1. Levenspiel O. and Kunii D., "Fluidization Engineering", John Wiley, 1972
2. Liang-Shih Fan, "Gas-Liquid-Solid Fluidization Engineering", Butterworths, 1989

**Course Outcomes:** At the end of the course, the student will be able to:

1. Performing and understanding the behavior of fluidization in fluidized bed
2. Evaluate the characterization of particles and power consumption in fluidization regimes
3. Understanding the applicability of the fluidized beds in chemical industries
4. Dispersion model, large solids in beds of smaller particles, staging of fluidized beds, Gas dispersion in beds.
5. Entrainment and elutriation, Mathematical model of a homogeneous fluidized bed.

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

## CH14C

## PROCESS PLANTS SIMULATION

Instruction: 3 hr/week

Credits: 3

Evaluation: 40+60

**Course Objectives;** Students will have to learn the following

- 1) Learn the Chemical Systems Modeling and Artificial Neural Networks
- 2) Understand how to design Steady State Extraction and Heat Conduction through Hollow Cylindrical, Unsteady State Mass Balance for CSTR and Heat Transfer in a Tubular Gas Pre Heater
- 3) Understand how to design models from Fluid Flow and Reaction Engineering
- 4) Develop Errors of Measurement, Problems in Data Regression and Solving Equation Solving and Modular Approach
- 5) Develop Algorithms based on Signal Flow Graph, Tearing Algorithms and Physical and Thermodynamic Properties of Convergence Promotion

### UNIT I

Modeling Aspects: Deterministic vs. Stochastic Processes, Physical modeling, Mathematical modeling, Chemical Systems Modeling, Cybernetics, Controlled System, Principles of Similarity

Classification of Mathematical Modeling: Independent and Dependent variables, Classification based on variation of independent variables, Classification based on state of the process, Classification based on type of the process, Boundary Conditions, The black Box Principle, Artificial Neural Networks

### UNIT II - Process Modeling-I

Models from mass transfer: steady state single stage solvent extraction, steady state two stage solvent extraction, steady state two stage cross current solvent extraction, , steady state N-stage solvent counter current extraction, unsteady state single stage solvent extraction, unsteady state mass balance in a stirred tank and in a mixing tank.

Models from Heat Transfer : steady state heat conduction through a hollow cylindrical pipe, unsteady state steam heating of a liquid, unsteady state heat loss through a measuring tank, heat transfer through extended surfaces, unsteady state heat transfer in a tubular gas pre heater

### UNIT III - Process Modeling-II

Models from fluid flow: flow through a packed bed column, flow of a film on the outside of a circular tube, annular flow with inner cylinder moving axially, flow between coaxial cylinders and concentric spheres

Models from Reaction Engineering : chemical reaction with diffusion in a tubular reactor, chemical reactor with heat transfer in a packed bed reactor, gas absorption accompanied by chemical reaction

## UNITIV

Error Propagation & Data Regression : Propagation of errors through addition, subtraction, multiplication and division, Errors of measurement, Precision errors, errors method

Data Regression : Theoretical properties, data regression methods, Problems in data regression

Process Simulation: Modular Approach, The equations solving approach

## UNITV

Decomposition of Networks : Tearing Algorithms, Algorithms based on signal flow graph and reduced digraph

Convergence Promotion: Newton's method, direct substitution method, Wegstein's method, dominant Eigenvalue method, quasi Newton method, Criterion for acceleration, Physical and Thermodynamic Properties

### TEXTBOOKS:

1. Process Plant Simulation, B. V. Babu, Oxford University press, 2004
2. Process Modeling, Simulation and Control for Chemical Engineers, 2<sup>nd</sup> ed., W. L. Luyben, McGraw-Hill, New York, 1990

### REFERENCE:

1. Introduction to Numerical Methods in Chemical Engineering, P. Ahuja, PHI, New Delhi, 2010
2. Process Modeling and Simulation, Amiya K. Jana, 2012.

**Course Objectives:** Students will be trained in

- 1) Modelling Aspects and Classification of Mathematical Modelling
- 2) How to Prepare Models from Mass Transfer and Model on Heat Transfer
- 3) How to Prepare Models from Fluid Flow and Model on Reaction Engineering
- 4) The analysis through Propagation of Errors, Error Methods, Data Regression Methods and Process Simulation
- 5) Decomposition of Networks and Convergence Promotion

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



## CH14C

## COMPUTATIONAL FLUID DYNAMICS

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives

1. To make students understand the governing equations of fluid dynamics and their derivation from laws of conservation
2. To develop a good understanding in computational skills, including discretisation, accuracy and stability.
3. To acquaint the students with a process of developing a mathematical and geometrical model of flow, applying appropriate boundary conditions and solving system of equations

### Unit I: Introduction to Fluid Dynamics

Concepts of Fluid Flow, Pressure distribution in fluids, Reynolds transport theorem, Integral form of conservation equations, Differential form of conservation equations, Different Types of Flows, Euler and Navier Stokes equations, Properties of supersonic and subsonic flows, Flow characteristics over various bodies. Philosophy of CFD, Governing equations of fluid dynamics and their physical meaning, Mathematical behavior of governing equations and the impact on CFD simulations, Simple CFD techniques and CFL condition. Numerical Methods in CFD: Finite Difference, Finite Volume, and Finite Element, Upwind and downwind schemes, Simple and Simpler schemes, Higher order methods, Implicit and explicit methods, Study and transient solutions

### Unit II : Grid Generation

Basic theory of structured grid generation, Surface grid generation, Monoblock, multiblock, hierarchical multi block, Moving and sliding multiblock, Grid clustering and grid enhancement. Basic theory of unstructured grid generation, advancing front, Delaunay triangulation and various point insertion methods, Unstructured quad and hex generation, grid based methods, various elements in unstructured grids, Surface mesh generation, Surface mesh repair, Volume grid generation, Volume mesh improvement, mesh smoothing algorithms, grid clustering and quality checks for volume mesh. Adaptive, Moving and Hybrid Grids, Need for adaptive and moving grids, Tet, pyramid, prism, and hex grids, using various elements in combination

### Unit III: Turbulence and its Modeling

Transition from laminar to turbulent flow, Effect of turbulence on time-averaged Navier-Stokes equations, Characteristics of simple turbulent flows, Free turbulent flows, Flat plate boundary layer and pipe flow, Turbulence models, Mixing length model, The k-ε model, Reynolds stress equation models, Algebraic stress equation models

### Unit IV: Chemical Fluid Mixing Simulation

Stirred tank modeling using the actual impeller geometry, Rotating frame model, The MRF Model Sliding mesh model, Snapshot model, Evaluating Mixing from Flow Field Results, Industrial Examples

## Unit IV: Post-Processing of CFD results

Contour plots, vector plots, and scatter plots, Shaded and transparent surfaces, Particle trajectories and path line trajectories, Animations and movies, Exploration and analysis of data.

### References

1. Anderson John D., "Computational Fluid Dynamics: The Basics with Applications", McGraw Hill, 1995
2. Ranade V.V., "Computational Flow Modeling for Chemical Reactor Engineering", Process Engineering Science, Volume 5, 2001
3. Knupp Patrick and Steinberg Stanly, "Fundamentals of Grid Generation", CRC Press, 1994
4. Wilcox D.C., "Turbulence Modelling for CFD", 1993
5. Wesseling Pieter, "An Introduction to Multigrid Methods", John Wiley & Sons, 1992
6. Thompson J.F., Warsi Z.U.A. and Mastin C.W., "Numerical Grid Generation: Foundations and Applications", North Holland, 1985
7. Patankar S.V., "Numerical Heat Transfer and Fluid Flow", McGraw-Hill, 1981
8. Gatski Thomas B., Hussaini M. Yousuff and Lumley John L., "Simulation and Modelling of Turbulent Flows", Oxford University Press, 1996
9. Laney, C.B., "Computational Gas Dynamics", Cambridge Uni. Press, 1998.

**Outcomes:** At the end of the course, the students will be able to:

1. Understand the basic principles of mathematics and numerical concepts of fluid dynamics.
2. Develop governing equations for a given fluid flow system.
3. Adapt finite difference techniques for fluid flow models.
4. Apply finite difference method for heat transfer problems.
5. Solve computational fluid flow problems using finite volume techniques. Get familiarized to modern CFD software used for the analysis of complex fluid-flow systems

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

## CH15C

## INDUSTRIAL POLLUTION CONTROL

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives

1. To understand the importance of industrial pollution and its abatement
2. To study the underlying principles of industrial pollution control
3. To acquaint the students with case studies
4. Students should be able to design complete treatment system

### Unit I: Industries & Environment

Industrial scenario in India - Industrial activity and Environment - Uses of Water by industry - Sources and types of industrial wastewater - Industrial wastewater and environmental impacts - Regulatory requirements for treatment of industrial wastewater - Industrial waste survey - Industrial wastewater generation rates, characterization and variables - Population equivalent - Toxicity of industrial effluents and Bioassay tests.

### Unit II: Industrial Noise pollution

Sources of noise pollution, characterization of noise pollution prevention & control of noise pollution, Factories Act 1948 for regulatory aspects of noise pollution.

### Unit III: Air Pollutant Abatement

Air pollutants scales of concentration, lapse rate and stability, plume behavior, dispersion of air pollutants, atmospheric dispersion equation and its solutions, Gaussian plume models. Air pollution control methods, Source correction methods, Design concepts for pollution abatement systems for particulates and gases. Such as gravity chambers, cyclone separators, filters, electrostatic precipitators, condensation, adsorption and absorption, thermal oxidation and biological processes.

### Unit IV: Wastewater treatment processes

Design concepts for primary treatment, grid chambers and primary sedimentation basins, selection of treatment process flow diagram, elements of conceptual process design, design of thickener, biological treatment Bacterial population dynamics, kinetics of biological growth and its applications to biological treatment, process design relationships and analysis, determination of kinetic coefficients, activated sludge process. Design, trickling filter design considerations, advanced treatment processes, Study of environment pollution from process industries and their abatement: Fertilizer, paper and pulp, inorganic acids, petroleum and petrochemicals, recovery of materials from process effluents.

### Unit V: Solid waste and Hazardous waste management

x Sources and classification, properties, public health aspects, Sanitary land fill design, Hazardous waste classification and rules, management strategies, Nuclear waste disposal Treatment methods - component separation, chemical and biological treatment, incineration, solidification and stabilization, and disposal methods, Latest Trends in solid waste management.

## References

1. Rao C.S., "Environmental Pollution Control Engineering", 2nd edition
2. Mahajan S.P., "Pollution Control in Process Industries".
3. Nemerow N.L., "Liquid waste of industry-theories, Practices and Treatment", Addison Wesley, New York, 1971
4. Weber W.J., "Physico-Chemical Processes for water quality control", Wiley Interscience New York, 1969
5. Strauss W., "Industrial Gas Cleaning", Pergamon, London, 1975
6. Stern A.C., "Air pollution", Volumes I to VI, academic Press, New York, 1968
7. Peterson and Gross. E.Jr., "Hand Book of Noise Measurement", 7th Edn, 2003.
8. Antony Milne, "Noise Pollution: Impact and Counter Measures", David & Charles PLC, 2009.

**Course Outcomes:** At the end of the course, the student will be able to:

1. Recognize the causes and effects of environmental pollution
2. Analyze the mechanism of proliferation of pollution
3. Develop methods for pollution abatement and waste minimization
4. Design treatment methods for gas, liquid and solid wastes
5. Nuclear waste disposal Treatment methods

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

## CH15C

## TRANSPORT IN POROUS MEDIA

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives:

1. Introduce the physics and governing mechanisms controlling flow and transport processes in porous media.
2. Learning Liquid and solute transport in porous media.

**Unit-I:** Fundamentals: Mass, momentum and energy transport, Darcy and Non-Darcy equations, equilibrium and non-equilibrium conditions, species transport, radioactive decay.

**Unit-II:** Effective medium approximation: equivalent thermal conductivity, viscosity, dispersion.

**Unit-III:** Exact solutions: Flow over a flat plate, flow past a cylinder, boundary-layers, reservoir problems.

**Unit-IV:** Special topics: Field scale and stochastic modeling, Turbulent flow, compressible flow, multiphase flow, numerical techniques, hierarchical porous media, nano scale porous media, multiscale modeling.

**Unit-V:** Engineering applications: Groundwater, waste disposal, oil and gas recovery, regenerators, energy storage systems. Experimental techniques: Flow visualization, quantitative methods, inverse parameter estimation.

### References:

1. Principles of Heat Transfer in Porous Media, by M. Kaviany, Springer New York (1995).
2. Transport Phenomena in Porous Media, Volumes I-III, edited by D.R. Ingham and I. Pop, Elsevier, New York (1998-2005).
3. Dynamics of Fluids in Porous Media, J. Bear, Dover (1988).
4. Introduction to Modeling of Transport Phenomena in Porous Media, J. Bear and Y. Bachmat, Kluwer Academic Publishers, London (1990).
5. Enhanced Oil Recovery, L.W. Lake, Gulf Publishing Co. Texas (1989).
6. The Mathematics of Reservoir Simulation, R.E. Ewing, SIAM Philadelphia (1983).
7. Stochastic Methods for Flow in Porous Media: Coping with Uncertainties, Zhang, D., Academic Press, California (2002).
8. The Method of Volume Averaging, S. Whitaker, Springer, New York (1999).

**Outcomes:** At the end of this course, students are able to:

1. Students will understand the mechanisms involved in transport processes in porous media and will be able to work with the equations that govern the fate and transport of gas, water and solutes in porous media.

## CH15C

## CHEMOINFORMATICS

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives

1. To give students a concept of Chemo-informatics related to chemical structure databases and database search methods
2. To understand the quantum methods and models involved in drug discovery and targeted drug delivery
3. To study the application of Chemical Libraries, Virtual Screening, Prediction of Pharmacological Properties

### Unit I : Chemo-informatics

Introduction, scope and application, Basics of Chemo-informatics, Current Chemo-informatics resources for synthetic polymers, pigments. Primary, secondary and tertiary sources of chemical information, Databases: Chemical Structure Databases (PubChem, Binding database, Drugbank), Database search methods: chemical indexing, proximity searching, 2D and 3D structure and substructure searching. Drawing the Chemical Structure: 2D & 3D drawing tools (ACD ChemsSketch) Structure optimization.

### Unit II: Introduction to quantum methods

Combinatorial chemistry (library design, synthesis and deconvolution), spectroscopic methods and analytical techniques, Representation of Molecules and Chemical Reactions: Different types of Notations, SMILES Coding, Structure of Mol files and Sd files (Molecular converter, SMILES Translator).

### Unit III: Analysis and use of chemical reaction information

Chemical property information, spectroscopic information, analytical chemistry information, chemical safety information, Drug Designing: Prediction of Properties of Compounds, QSAR Data Analysis, Structure-Activity Relationships, Electronic properties, Lead Identification, Molecular Descriptor Analysis.

### Unit IV: Target Identification

Molecular Modeling and Structure Elucidation: Homology Modelling (Modeller 9v7, PROCHECK), Visualization and validation of the Molecule (Rasmol, Pymol Discovery studio), Applications of Chemoinformatics in Drug Research - Chemical Libraries, Virtual Screening, Prediction of Pharmacological Properties.

### Unit V: Drug Discovery

Structure based drug designing, Docking Studies (Target Selection, Active site analysis, Ligand preparation and conformational analysis, Rigid and flexible docking, Structure based design of lead compounds, Library docking), Pharmacophore - Based Drug Design, Pharmacophore Modeling (Identification of pharmacophore features, Building 2D/3D pharmacophore hypothesis), Toxicity Analysis - Pharmacological Properties (Absorption,

Distribution and Toxicity), Global Properties (Oral Bioavailability and Drug-Likeness) (ADME, OSIRIS, and MOLINSPIRATION)

## References

1. Bajorath J (2004), "Chemoinformatics: Concepts, Methods and Tools for Drug Discovery" Humana Press
2. Leach A, Gillet V, "An Introduction to Chemoinformatics" Revised edition, Springer
3. Gasteiger J, Engel T. "A text book of Chemoinformatics" Wiley-VCH GmbH & Co. KGaA
4. Bunin B, Siesel B, Guillermo M. "Chemoinformatics: Theory, Practice & Products", Springer
5. Lavine B. (2005), "Chemometrics and Chemoinformatics", American Chemical Society
6. Gasteiger J. and Engel T (2003) "Chemoinformatics" Wiley-VCH
7. Bunin Barry A, Siesel Brian, Morales Guillermo, Bajorath Jürgen. Chemoinformatics: Theory, Practice, & Products Publisher: New York, Springer. 2006.
8. Leach Andrew R., Valerie J. Gillet, "An introduction to Chemoinformatics", Publisher: Kluwer academic, 2003. ISBN: 1402013477
9. Gasteiger Johann, Handbook of Chemoinformatics: From Data to Knowledge (4 Volumes),  
2003. Publisher: Wiley-VCH.

**Course Outcomes:** At the end of the course, the student will be able to:

1. The course will introduce the students preparing for professional work in chemistry must learn how to retrieve specific information from the enormous and rapidly expanding chemical literature.
2. The course will provide a broad overview of the computer technology to chemistry in all of its manifestations.
3. The course will expose the student to current and relevant applications in QSAR and Drug Design.

## CH15C

## ADVANCED CONTROL SYSTEMS

Instruction: 3 hr/week

Credits: 3

Evaluation: 40+60

**Course Educational Objectives;** Students will have to learn the following

- 1) Learn the Concepts of Advanced Control Strategies
- 2) Understand the Multi Input and Multi Output controlling
- 3) Understand the Purpose of Digital Data Acquisition and Control
- 4) Develop Discrete Time Models & Their Dynamic Response
- 5) Design the Digital Controllers

### **Unit I:**

**Feed Forward and Ratio Control** – Introduction, Feed forward controller design based on steady state and dynamic models, tuning and configuration of feed forward control

**Advanced Control Strategies**– Cascade control, time delay compensation and inferential control, selective and override systems, adaptive control, statistical process control

### **Unit II:**

**Control of Multi Input, Multi-Output Systems**– Process interactions and control loop interactions, pairing of controlled and manipulated variables, strategy for reducing interactions, decoupling, multivariable control techniques

**Supervisory Control**– Basic requirements, applications, formulation and solution of optimization problems, unconstrained and constrained optimization

### **Unit III:**

**Digital Computer Control**– Digital control systems in process control, distributed instrumentation and control systems, general purpose digital data acquisition, digital control hardware and software, table driven PID controller, Programmable logic controllers and batch process control

**Sampling and Filtering of Continuous Measurements**– Sampling and signal reconstruction, selection of sampling period, signal processing and data filtering, comparison of analog and digital filters, effect of filter selection on control system performance

### **Unit IV:**

**Development of Discrete Time Models** – Finite difference models, exact discretization for linear systems, higher order systems, fitting discrete time equations to process data

**Dynamic Response of Discrete-Time Systems**– The z-Transform, inversion, pulse transfer function, relating pulse transfer functions to difference equations, effect of pole and zero locations, conversion between laplace and z- transforms



## **UnitV:**

**Analysis of Sampled – Data Control Systems**– Open loop block diagram analysis, development of closed loop transfer functions, stability of sampled data control systems

**Design of Digital Controllers**– Digital PID controller, selection of controller parameters, direct synthesis methods, digital feed forward control, combined load estimation and time delay compensation

### **TextBooks:**

1. ProcessDynamicsandControl–D.E.Seborg,T.F.EdgarandD.A.Mellichamp, John Wiley & Sons
2. ChemicalProcesscontrol–AnIntroductiontoTheoryandPractice-George Stephanopoulos, Prenticehall1990.

**CourseObjectives:**Studentswillbeabletounderstandandanalyze

- 1) FeedForward,RatioControlsandAdvancedControllers
- 2) ControlLoopInteractions&Optimization
- 3) DigitalComputerControl, selectionofsamplingperiod,comparisonofanaloganddigital filters
- 4) FiniteDifferenceModels,Z-Transforms,PulseTransferFunctions
- 5) SamplesandDataControlSystems

II SEMESTER

## CH21C

## MEMBRANE SEPARATIONS

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

**Course Educational Objectives;** Students will have to learn the following

- 1) Learn the Properties of Membrane and Types of Membrane
- 2) Learn the Types of Filtrations used
- 3) Design Reverse Osmosis Module
- 4) Learn Gas Separation and Pervaporation
- 5) Understand different Membrane Processes

### UNIT I :

#### **OverView of Membrane Separations**

**Membrane Types, Materials, Preparation and Characterization-** Types of Synthetic Membranes – Membrane Modules – Typical Flow patterns – Membrane materials – Pore Characteristics – Membrane Manufacture – Measurement of Pore size and Solute rejection Properties – surface Properties measurement and interpretation

### UNIT II :

**Nano Filtration-** principles – nano-filtration membranes – Mass Transfer – Process Limitations – Industrial application

**Ultrafiltration -**Basic Principles – Membranes – Configuration – Types of Devices – Factors affecting performance – Flux – Models for Solvent Flux – Fouling and Flux decline – Methods to reduce Concentration Polarization – Energy Considerations – Micellar enhanced UF – Affinity UF – Applications

**Microfiltration-** Basic Principles – Membranes – Transport Mechanism – retention characteristics – Flow Characteristics – Membrane Plugging and Throughput – Fouling – energy Considerations – Applications

### UNIT III:

**Reverse Osmosis-** Concepts – Phenomenon of RO – Models for RO transport – Design and Operating parameters – Concentration Polarization – Membrane plugging – Equivalent work requirement – Design of an RO module – RO of non-aqueous systems – Osmotic pin cell effect – Forward osmosis – Applications

**Dialysis-** Principles – Dialysis systems – Membranes – Mass transfer – Applications – Diffusion dialysis

### UNIT IV:

**Gas Separation-** Basic Principles – Membranes – Membrane Modules – Fundamental Mechanisms of Gas Transport – Factors affecting Gas Permeation – Complete Mixing Model – Cross and Countercurrent models – Applications

**Pervaporation-** Basic Principles – Advantages – Membrane characteristics – Thermodynamic Considerations – Mass transfer – Thermodynamic Considerations – Design of a Module – Concentration Polarization – factors affecting pervaporation – Temperature drop at the interface – Applications

## UNITV:

**IonExchange Membrane Process**-Basic Principles – Ion exchange Membranes – Energy requirement, Efficiency- Concentration Polarization and limiting current density – Other operating parameters – applications

**Liquid Membranes**- Types of liquid membranes – Mechanism of Mass transfer – Applications

**Other Membrane Processes**– Membrane contactor and applications – Membrane distillation – Membrane reactors – PEM Hydrogen Fuel Cell

## TextBook

1. MembraneSeparationProcesses–Kaushiknath–PrenticeHall,2008

## References

1. ReverseOsmosisandSyntheticMembranesTheory,TechnologyandEngineering, Sourirajan,S National Research Council, Canada.
2. Reverse Osmosis/ Ultrafiltration Process Principles, Sourirajan,S. and Matsuura, T., NationalResearchCouncil,Canada.SeparationProcesses,ElsevierScientificPublication.
3. IndustrialMembraneSeparationTechnology,Scott,K.,andHughes,R.(Eds.),Blackie Academic & Professional London.
4. SeparationProcesses,King,C.J, TataMcGrawHill,NewDelhi.
5. MembraneProcesses,Rautenbatch,R.,andAlbrecht,RJohnWiley&Sons,NewYork.
6. MembraneSeparationProcesses, Baum,B.,Halley,W.andWhite,R.A,Elsevier Scientific Publication

## CourseObjectives:Studentsgain

- 1) KnowledgeonPreparationandCharacterizationofMaterialsandTypesofMembrane
- 2) KnowledgeonNano-Filtration,Ultra-FiltrationandMicro-Filtration
- 3) KnowledgeonDesigningReverseOsmosisandDialysis
- 4) ConceptsofGasSeparationandPervaporationandDesignofPervaporationModule
- 5) KnowledgeonIonExchangeMembraneProcess,LiquidMembranesandOther Membrane Processes

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

**CH22C****OPTIMIZATION THEORY & PRACTICE**

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

**Course Educational Objectives:**

- 1) To learn problem formulation and basic concepts of optimization.
- 2) To study the numerical methods to solve single variable unconstrained problems
- 3) To understand and apply numerical methods to solve unconstrained multi-variable problems
- 4) To learn linear & non-linear programming methods
- 5) To know the applications of optimization through different examples

**Unit-I: Introduction**

Basic concepts of optimization, applications of optimization, general procedure for solving optimization problem, formulation of the objective function, fitting models to data, classification of functions.

**Unit-II: Single Variable unconstrained optimization methods**

Direct search methods-Interval halving method, Fibonacci method, Golden section method; Direct root methods-Newton method and Quasi Newton method; Polynomial approximation methods-Quadratic interpolation and cubic interpolation.

**Unit-III: Optimization of unconstrained multivariable functions**

Direct search methods-random search, grid search, uni-variate search and pattern search methods.; Indirect search methods -steepest descent, conjugate gradient methods, Newton's method and secant method.

**Unit-IV: Linear and non-linear programming**

Linear programming: Basic concepts in linear programming, Standard LP form, Graphical solution and Simplex method.

Non-linear programming: Lagrange multiplier method, Quadratic programming, Penalty function and augmented Lagrangian methods.

**Unit-V: Applications of optimization**

Optimizing recovery of waste heat, optimal design and operation of a conventional staged-distillation column, optimal pipe diameter, optimal residence time for maximum yield in chemostat and optimization of a thermal cracker using linear programming.

**Text Book:**

1. Edgar, T.F., Himmelblau, D.M. and Ladson, L.S., "Optimization of Chemical Processes", 2nd Ed., McGraw Hill, New York.

**ReferenceBooks:**

1. Diwaker,U.W.“IntroductiontoAppliedOptimization”,Kluwer.
2. Joshi,M.C.andMoudgalya,K.M.,“Optimization,TheoryandPractice”,Narosa, New Delhi, 2004.
3. Rao,S.S.,EngineeringOptimization:TheoryandPractice, NewAgePublishers.

**CourseOutcomes:**Studentwillbeableto

- 1) formulateandanalysetheoptimizationofthegivenphysicalsituation.
- 2) Applydifferentmethodsofoptimizationandtosuggestatechniqueforspecificproblem
- 3) Understandthedifferencebetweenconstrainedandunconstrainedoptimization
- 4) Understandtheimportanceoflinearprogrammingproblems
- 5) Realizetheimportanceofoptimizationbyunderstandingdifferentexamples

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>	<b>PO8</b>	<b>PO9</b>	<b>PO10</b>	<b>PO11</b>	<b>PO12</b>
CO1		1	1	1				1	1			
CO2		2	1	1				2	1			
CO3		1	1	1		2	1	1	1			
CO4		2	1	1				2	1			
CO5		2	2	1				1	1			

**CH25L****STEADY STATE SIMULATION LAB****II Semester**

Instruction, hours/week: 3

Assessment: 40+60

To introduce students to use of software packages for simulation and also analyzing flow sheets

1. Introduction of Software packages.
2. Setting up models for simulation.
3. Flowsheeting concepts.
4. Steady state simulation for generation of VLE data.
5. Steady state simulation for conversion calculation for single and multiple reactions
6. Steady state simulation for heat and cooling duty of heat exchangers.
7. Simulation of flash column.

**CH26L****ADVANCED INSTRUMENTATION LAB**

Instruction, hours/week: 3

Assessment: 40+60

To introduce students to use of new Analytical Instruments for analysis like UV Spectro Photo meter, HPLC, Atomic Adsorption Spectro Photometer etc.

## INDUSTRIAL SAFETY

**Unit-I:** Industrial safety: Accident, causes, types, results and control, mechanical and electrical hazards, types, causes and preventive steps/procedure, describe salient points of factories act 1948 for health and safety, wash rooms, drinking water layouts, light, cleanliness, fire, guarding, pressure vessels, etc, Safety color codes. Fire prevention and firefighting, equipment and methods.

**Unit-II:** Fundamentals of maintenance engineering: Definition and aim of maintenance engineering, Primary and secondary functions and responsibility of maintenance department, Types of maintenance, Types and applications of tools used for maintenance, Maintenance cost & its relation with replacement economy, Service life of equipment.

**Unit-III:** Wear and Corrosion and their prevention: Wear- types, causes, effects, wear reduction methods, lubricants-types and applications, Lubrication methods, general sketch, working and applications, i. Screw down grease cup, ii. Pressure grease gun, iii. Splash lubrication, iv. Gravity lubrication, v. Wick feed lubrication vi. Side feed lubrication, vii. Ring lubrication, Definition, principle and factors affecting the corrosion. Types of corrosion, corrosion prevention methods.

**Unit-IV:** Fault tracing: Fault tracing-concept and importance, decision tree concept, need and applications, sequence of fault finding activities, show as decision tree, draw decision tree for problems in machine tools, hydraulic, pneumatic, automotive, thermal and electrical equipment's like, I. Any one machine tool, ii. Pump iii. Air compressor, iv. Internal combustion engine, v. Boiler, vi. Electrical motors, Types of faults in machine tools and their general causes.

**Unit-V:** Periodic and preventive maintenance: Periodic inspection-concept and need, degreasing, cleaning and repairing schemes, overhauling of mechanical components, overhauling of electrical motor, common troubles and remedies of electric motor, repair complexities and its use, definition, need, steps and advantages of preventive maintenance. Steps/procedure for periodic and preventive maintenance of: I. Machine tools, ii. Pumps, iii. Air compressors, iv. Diesel generating (DG) sets, Program and schedule of preventive maintenance of mechanical and electrical equipment, advantages of preventive maintenance. Repair cycle concept and importance

### Reference:

1. Maintenance Engineering Handbook, Higgins & Morrow, Da Information Services.
2. Maintenance Engineering, H.P. Garg, S. Chand and Company.
3. Pump-hydraulic Compressors, Audels, McGraw Hill Publication.
4. Foundation Engineering Handbook, Winterkorn, Hans, Chapman & Hall London.



## **CH23C            MODERN CONCEPTS IN CATALYSIS AND SURFACE PHENOMENON**

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### **Objectives**

1. To give the students insight into advances in catalytic reaction engineering
2. To understand the mechanisms involved in catalytic reactions
3. To study the catalyst characterization techniques
4. To study the advanced industrial applications in catalysis
5. To understand the principles behind catalyst deactivation and study their models

### **Unit I : Introduction to Catalysis**

Definition of Catalytic activity, Magnitude of Turnover Frequencies and Active Site Concentrations, Evolution of Important Concepts and Techniques in Heterogeneous Catalysis, Classification of Catalysts – Homogeneous, Heterogeneous, Biocatalysts, Dual Functional Catalysts, Enzymes, Solid Catalysts, Powder Catalysts, Pellets, Composition, Active Ingredients, Supportive materials, Catalysts Activation, Catalyst Deactivation.

### **Unit II: Adsorption in Catalysis**

Adsorption and its importance in Catalysis, Adsorption and potential energy curves, Surface Reconstruction, Adsorption Isotherms and Isobars, Dynamical Considerations, Types of Adsorption Isotherms and their Derivation from Kinetic Principles, Mobility at Surfaces, Kinetics of surface Reactions, Photochemistry on oxide and metallic surfaces, Characterization of the adsorbed molecules

### **Unit III: Catalyst Characterization**

Catalyst Characterization Methods – Their Working Principle and Applications – XRF, XRD, IR Spectroscopy, XPS, UPS, ESR, NMR; Infrared, Raman, NMR, Mossbauer and X-Ray Absorption spectroscopy, Surface Acidity and Toxicity, Activity, Life time, Bulk density, Thermal stability Crystal Defects, Perovskites, Spinels, Clays, Pillared Clays, Zeolites

### **Unit IV: Significance of Pore Structure and Surface Area**

Importance of Surface Area and Pore Structure, Experimental Methods for Estimating Surface Area – Volumetric, Gravimetric, Dynamic Methods, Experimental Methods for Estimating Pore Volume and Diameter – Gas Adsorption and Mercury Porosimeter Method, Models of the Pore Structure – Hysteresis Loops, Geometric Models, Wheeler's Model, Dusty Gas Model, Random Pore Model, Diffusion in Porous Catalysts – Effective Diffusivity, Knudsen Diffusion, Effect of Intraparticle Diffusion, Non-isothermal Reactions in Pores, Diffusion Control.

### **Unit V: Industrial applications – Case Studies**

Industrial processes involving heterogeneous solid catalyst: Synthesis of Methanol, Fischer-Tropsch Catalysis, Synthesis of Ammonia, Automobile Exhaust Catalysts and Catalyst Monolith, Photocatalytic Breakdown of Water and the Harnessing of Solar Energy.

Contribution of homogeneous catalytic process in chemical industry: Oxidations of Alkenes such as production of acetaldehyde, propylene oxide etc., Polymerization such as production of polyethylene, polypropylene or polyester production

### References

1. Emmett, P.H. - "Catalysis Vol. I and II, Reinhold Corp.", New York, 1954
2. Smith, J.M. - "Chemical Engineering Kinetics", McGraw Hill, 1971
3. Thomas and Thomas - "Introduction to Heterogeneous Catalysts", Academic Press, London 1967
4. Piet W.N.M. van Leeuwen, Homogeneous catalysis: Understanding the Art, Springer, 2004
5. Piet W.N.M. van Leeuwen, and John C. Chadwick, Homogeneous catalysis: Activity-stability - deactivation, Wiley, VCH, 2011.

**Course Outcomes:** At the end of the course, the student will be able to:

1. To understand the concepts of homogeneous and heterogeneous catalysis, with specific examples.
2. To study reaction mechanisms and kinetics of homogeneous and heterogeneous catalytic reactions.
3. To familiarize with the characterization of catalysts
4. To understand the application and mechanisms of several types of catalysts in chemical industry.

## CH22C

## ADVANCED DOWNSTREAM PROCESSING

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives

1. To understand the unit processes involved in downstream processing.
2. To study advanced treatment methods.
3. To study the energy conservation in different separation processes
4. To understand the underlying design principles

### Unit I: Introduction]

Introduction to Downstream processes theory, applications in chemical separation for Gas-Liquid system, Gas-Solid system. Super critical fluids extraction in food, pharmaceutical, environmental and petroleum applications, water treatment, desalination, Bio separation, dialysis, industrial dialysis.

### Unit II: Downstream Processes in Petrochemical Industry

Cryogenic distillation for refinery, petrochemical off gases, natural gases, gas recovery-Olefin, Helium, Nitrogen, Desulfurization - coal, flue gases

### Unit III: Advanced Distillation Processes

Azeotropic & extractive distillation - residue curve maps, homogeneous azeotropic distillation, pressure swing distillation, Column sequences, heterogeneous azeotropic distillation.

### Unit IV: Energy conservation in separation processes

Energy balance, molecular sieves - zeolites, adsorption, catalytic properties, manufacturing processes, hydrogel process, application, New trends.

### Unit IV: Non-Ideal Mixtures and Ion Exchange

Separations process synthesis for nonazeotropic mixtures, non ideal liquid mixtures, separation synthesis algorithm, Ion exchange - manufacture of resins, physical & chemical properties, capacity, selectivity, application, regeneration, equipment, catalysis use.

### References

1. Perry's "Chemical Engg. Handbook": McGraw Hill Pub.
2. Douglas J.M., "Conceptual Design of Chemical Processes", McGraw Hill
3. Liu Y.A., "Recent Developments in Chemical Process & Plant Design", John Wiley & Sons Inc.
4. Timmerhaus K.D., "Cryogenic Process Engg.", Plenum Press
5. Othmer Kirk "Encyclopedia of Separation Technology, Vol I & II", Wiley Interscience

**Course Outcomes:** At the end of the course, the student will be able to:

1. To learn effective strategies of downstream processing in chemical industry.
2. Understand the role of downstream processing.
3. Analyze reactors, upstream and downstream processes in production

## CH23C

## PROCESS SYNTHESIS & ANALYSIS

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Course Objectives:

- 1) To familiarize the students about various economic aspects of chemical processes
- 2) To learn basics of cost estimation and to understand the time value of money
- 3) To learn the importance of cash flow diagrams and break-even analysis.
- 4) To study depreciation methods and methods of estimation of profitability of an industry
- 5) To study about heat exchange networks.

### UNIT-I:

**Nature of Process Synthesis & Analysis :** Creative aspects – A hierarchical approach

**Engineering Economics :** Cost Information – Estimation of Capital and Operating Costs – Total Capital Investment - Total Product Cost - Time Value of Money – Measures of Process Profitability – Simplifying the Economic Analysis for Conceptual Design

### UNIT II :

**Economic Decision Making :** Solvent Recovery System – Problem Definition & General Considerations – Design of a Gas Absorber – Equipment Design Consideration – Rules of Thumb

**Input Information & Batch- Continuous:** Input Information – Level 1 Decision – Batch Vs. Continuous

### UNIT III:

**Input-Output Structure of the Flow Sheet :** Decisions for the I/O structure – Design Variables – Overall Material Balances – Stream Costs – Process Alternatives

**Recycle Structure of the Flow Sheet :** Decisions determining the recycle Structure – Recycle Material balances – reactor Heat Effects – Equilibrium Limitations – Compress Design & Costs – Reactor Design – recycle Economic Evaluation

### Unit IV:

**Heat Exchanger Networks** – Minimum Heating & Cooling Requirements – Minimum Number of Exchangers – Area Estimates – Design of Minimum Energy Heat Exchanger Networks – Loops and Paths – Reducing the Number of Exchanger – Stream Splitting – Heat and Power Integration – Heat Distillation – HAD Process

### UNIT V:

**Separation System :** General Structure – Vapor Recovery System – Liquid Separation System – Azeotropic Systems – Rigorous Material Balances

**Cost Diagrams and Quick Screening of Process Alternatives** - Cost Diagrams for simple and complex process – Quick Screening of Process Alternatives – HAD Process

### Text Book:

1. Conceptual Design of Chemical Processes, Douglas, J.M., McGraw Hill,

**Reference Books:**

1. Chemical Process Design, Robin Smith, McGraw Hill,
2. Chemical Process Design, Dimian A.C. & Bidea, C.S., Wiley-VCH, 2008
3. Chemical Process Synthesis & Engineering Design, Kumar, A, Tata McGraw Hill, 1982
4. Systematic Methods of Chemical Process Design, Biegler, L.T., Grossman, E.I and Westerberg, A.W. Prentice Hall Inc.
5. Product and Process Design Principles, Seider, W.D., Seider, J.D & Lewin, D.R. Wiley, 2005

**Course Outcomes:** Student will be able to

- 1) understand the concepts of Engineering economics
- 2) Able to estimate various costs involved in a process industry and evaluate the tax burden of an establishment
- 3) Able to estimate profitability of a company
- 4) Understand the heat exchanger networks and their importance in industry
- 5) Compute breakeven period for an investment and rate of return

## CH23C

## MICROANDNANOFLUIDICS

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives:

1. To introduce to the students, the various opportunities in the emerging field of micro and nano fluids.
2. To make students familiar with the important concepts applicable to small micro and nano fluidic devices, their fabrication, characterization and application
3. To get familiarized with the new concepts of real-time nanomanipulation &

**Unit-1:** Introduction: Fundamentals of kinetic theory-molecular models, micro and macroscopic properties, binary collisions, distribution functions, Boltzmann equation and Maxwellian distribution functions-Wall slip effects and accommodation coefficients, flow and heat transfer analysis of micro scale Couette flows, Pressure driven gas micro-flows with wall slip effects, heat transfer in micro-Poiseuille flows, effects of compressibility. Pressure Driven Liquid Micro flow: apparent slip effects, physics of near-wall micro scale liquid flows, capillary flows, electro-kinetically driven liquid micro - flows and electric double layer (EDL) effects, concepts of electro osmosis, electrophoresis and dielectrophoresis.

**Unit- 2:** Laminar flow: Hagen-Poiseuille eqn, basic fluid ideas, Special considerations of flow in small channels, mixing, microvalves & micropumps, Approaches toward combining living cells, microfluidics and 'the body' on a chip, Chemotaxis, cell motility. Case Studies in Microfluidic Devices. Ionic transport: Polymer transport – microtubule transport in nanotube channels driven by Electric Fields and by Kinesin Biomolecular Motors - Electrophoresis of individual nanotubules in microfluidic channels.

**Unit-3:** Fabrication techniques for Nanofluidic channels – Bio molecules separation using Nanochannels - Biomolecules Concentration using Nano channels – Confinement of Bio molecules using Nano channels. Hydrodynamics: Particle moving in flow fields – Potential Functions in Low Reynolds Number Flow – Arrays of Obstacles and how particles Move in them: Puzzles and Paradoxes in Low Re Flow.

**Unit-4:** Micro fluidics and Lab-on-a-chip: Microfluidic Devices - Microchannels, Micro filters, Microvalves, Micropumps, Microneedles, Microreservoirs, Micro-reaction chambers. Concepts and Advantages of Microfluidic Devices - Fluidic Transport - Stacking and Scaling – Materials for The Manufacture (Silicon, Glass, Polymers) - Fluidic Structures - Fabrication Methods - Surface Modifications - Spotting - Detection Mechanisms. Microcontact printing of Proteins Strategies-printing types- methods and characterization- Cell nanostructure interactions-networks for neuronal cells. Applications in Automatic DNA sequencing, DNA and Protein microarrays.

**Unit-5:** BioMEMS (Micro-Electro-Mechanical Systems): Introduction and Overview, Biosignal Transduction Mechanisms: Electromagnetic Transducers Mechanical Transducers, Chemical Transducers, Optical Transducers – Sensing and Actuating mechanisms (for all types). Case Studies in Biomagnetic Sensors, Applications of optical and chemical transducers. Ultimate Limits of Fabrication and Measurement, Recent Developments in BioMEMS and BioNEMS - An alternative approach to traditional surgery, Specific targeting of tumors and other organs for drug delivery, Micro-visualization and manipulation,

Implantation of microsensors, microactuators and other components of a larger implanted device or external system (synthetic organs).

### **Text Books**

1. Joshua Edel "Nanofluidics" RSC Publishing, 2009.
2. Patric Tabeling "Introduction to Microfluids" Oxford U. Press, New York 2005.
3. K. Sarit "Nano Fluids; Science and Technology", RSC Publishing, 2007.

### **References**

1. M. Madou, Fundamentals of Microfabrication, CRC Press, 1997
2. G. Kovacs, Micromachined Transducers, McGraw-Hill, 1998
3. Steven S Saliterman, Fundamentals of BioMEMS and Medical Microdevices, 2006

**Outcomes:** At the end of this course, students are able to:

1. Introduce students to the physical principles to analyze fluid flow in micro and nano-sized devices. It unifies the thermal sciences with electrostatics, electrokinetics, colloid science; electrochemistry; and molecular biology.

**CH24C****PHASE TRANSITIONS IN PROCESS EQUIPMENT**

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

**Objectives:**

1. Basic laws in thermodynamics.
2. Basic statistical concepts and methods: heat, work, energy, temperature and the kinetic theory of matter; entropy, ensemble, partition function, etc
3. Learning phase transition catalysis
4. Have a good grasp of the basic thermodynamic interactions and process: adiabatic, isothermal, etc

**Unit-I:** Thermodynamic aspects of phase transitions: Concept of phase, First-order phase transition, conditions for phase coexistence lines, free energy barrier of nucleation, and crystal-melt interfacial free energy, Ehrenfest classification of phase transitions, Van der Waals equation of state, Critical point

**Unit-II:** Single phase and multiphase catalytic reactions, Acid-base catalysis, Transition metal catalysis, Phase transfer catalysis, Micellar catalysis, Microemulsion catalysis, Electron transfer catalysis, Heteropoly acid catalysis, Homogeneous polymer catalysis, Heterogenisation of homogeneous catalysts.

**Unit-III:** Applications to Multi-phase Systems Stability conditions for a homogeneous system, equilibrium between phases, phase transformations, general relations for a system with several components, general conditions for chemical equilibrium, chemical equilibrium between ideal gases, and the equilibrium constants in terms of partition functions.

**Unit-IV:** Phase diagrams and transformations Phase rule - single and binary phase diagrams, lever rule, microstructural changes during cooling, Al<sub>2</sub>O<sub>3</sub>, Cr<sub>2</sub>O<sub>3</sub>, Pb-Sn, Ag-Pt and Fe-Fe<sub>3</sub>C Systems phase diagrams, phase transformations, corrosion-theories of corrosion, control and prevention of corrosion

**UNIT-V:** Energy balance - heat capacity and calculation of enthalpy changes, Enthalpy changes for phase transitions, evaporation, Clausius - Clapeyron equation,

**References:**

1. Hegedus, L.S., Transition Metals in the Synthesis of Complex Organic Molecules, University Science Book (2010) 3rd ed.
2. Raghavan V., Material Science and Engineering Prentice Hall of India, 1996
3. David M. Himmelblau, "Basic principles and calculations in chemical engineering", Prentice Hall of India Ltd., 6th Edition, 1998.
4. A. Hougen, K.M. Watson and K.A. Ragatz, "Chemical Process Principles", Vol 1, John Wiley, 1960.



**Outcomes:** At the end of this course, students are able to:

1. The student is expected to obtain considerable insight into various types of phase transitions, and how these can be described theoretically in different ways
2. Predict relationships between physical quantities using the laws and methods of thermodynamics.
3. Find probabilities and thermal quantities (free energy, entropy, etc) given the energy eigen values of a system.
4. The student is expected to obtain considerable insight into various types of phase transitions, and how these can be described theoretically in different ways
5. Predict relationships between physical quantities using the laws and methods of thermodynamics.
6. Find probabilities and thermal quantities (free energy, entropy, etc) given the energy eigen values of a system.

## CH24C

## PROCESS INTENSIFICATION

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives:

1. Understand the concept of Process Intensification.
2. Know the limitations of intensification of the chemical processes.
3. Apply the techniques of intensification to a range of chemical processes.
4. Develop various process equipment used for intensifying the processes.
5. Infer alternative solutions keeping in view point, the environmental protection, economic viability and social acceptance.

**Unit-I:** 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, Techniques for PI application.

**Unit-II:** Process Intensification through microreaction technology: Effect of miniaturization on unit operations and reactions, Implementation of Microreaction Technology, From basic Properties To 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.

**Unit-III:** 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, High reactors.

**Unit-IV:** 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: Absorption of NO<sub>x</sub> 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.

**Unit-V:** 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, Sonocrystallization, Reactive separations, Supercritical fluids

**References:**

1. Stankiewicz, A. and Moulijn, (Eds.), Reengineering the Chemical Process Plants, Process Intensification, Marcel Dekker, 2003.
2. Reay D., Ramshaw C., Harvey A., Process Intensification, Butterworth-Heinemann, 2008.
3. Kamelia Boodhoo (Editor), Adam Harvey (Editor), Process Intensification Technologies for Green Chemistry: Engineering Solutions for Sustainable Chemical Processing, Wiley, 2013.
4. Segovia-Hernández, Juan Gabriel, Bonilla-Petriciolet, Adrián (Eds.) Process Intensification in Chemical Engineering Design Optimization and Control, Springer, 2016.
5. Reay, Ramshaw, Harvey, Process Intensification, Engineering for Efficiency, Sustainability and Flexibility, Butterworth-Heinemann, 2013.

**Outcomes:** At the end of this course, students are able to:

1. Assess the values and limitations of process intensification, cleaner technologies and waste minimization options.
2. Measure and monitor the usage of raw materials and wastes generating from production and frame the strategies for reduction, reuse and recycle.
3. Obtain alternative solutions ensuring a more sustainable future based on environmental protection, economic viability and social acceptance.
4. Analyzed data, observe trends and relate this to other variables.
5. Plan for research in new energy systems, materials and process intensification.

**CH24C****MICROFLOW CHEMISTRY AND PROCESS TECHNOLOGY**

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

**Objectives:**

1. Introduce the student to microflow chemistry and process technology.
2. Learning Micromixers, Mixing Principles.
3. Learning microreactor based chemicals production

**Unit-I:** State of the Art of Micro reaction Technology, Structural Hierarchy of Micro reactors, Functional Classification of Micro reactors, Fundamental Advantages of Micro reactors, Advantages of Micro reactors Due to Decrease of Physical Size, Advantages of Micro reactors Due to Increase of Number of Units, Potential Benefits of Microreactors

**Unit-II:** Modern Micro fabrication Techniques for Micro reactors, Evaluation of Suitability of a Technique, Anisotropic Wet Etching of Silicon, Dry Etching of Silicon, LIGA Process, Injection Molding, Wet Chemical Etching of Glass, Advanced Mechanical Techniques

**Unit-III:** Micro mixers, Mixing Principles and Classes of Macroscopic Mixing Equipment, Mixing Principles and Classes of Miniaturized Mixers, Mixing Tee-Type Configuration

**Unit-IV:** Microsystems for Gas Phase Reactions, Catalyst Supply for Microreactors, Types of Gas Phase Micro reactors, Micro channel Catalyst Structures, H<sub>2</sub>/O<sub>2</sub> Reaction, Selective Partial Hydrogenation of Benzene, Selective Oxidation of 1-Butene to Maleic Anhydride, Selective Oxidation of Ethylene to Ethylene Oxide, Oxidative Dehydrogenation of Alcohols, Synthesis of Methyl Isocyanate and Various Other Hazardous Gases, Synthesis of Ethylene Oxide, Oxidation of Ammonia

**Unit-V:** Microsystems for Energy Generation, Micro devices for Vaporization of Liquid Fuels, Micro devices for Conversion of Gaseous Fuels to Syngas by Means of Partial Oxidations, Hydrogen Generation by Partial Oxidations, Micro devices for Conversion of Gaseous Fuels to Syngas by Means of Steam Reforming

**References:**

1. Wolfgang Ehrfeld, Volker Hessel, Holger Löwe Microreactors New Technology for Modern Chemistry © WILEY-VCH Verlag GmbH, D-69469 Weinheim (Federal Republic of Germany), 2000.
2. S.V. Luis and E. Garcia-Verdugo, Chemical Reactions and Processes under Flow Conditions, University Jaume I/CSIC, Castellón, Spain, The Royal Society of Chemistry 2010
3. Madhvanand N. Kashid, Albert Renken, and Liubov Kiwi-Minsker, Microstructured Devices for Chemical Processing, Wiley-VCH Verlag GmbH & Co. KGaA, Boschstr ©2015 12, 69469 Weinheim, German.
4. Hessel, V., Renken, A., Schouten, J.C., Yoshida, Micro Process Engineering "A Comprehensive Handbook 2009, ISBN 978-3-527-31550-5.

**Outcomes:** At the end of this course, students are able to:

1. Students will understand the role of microflow chemistry and process technology in chemical engineering.
2. The student is expected to obtain considerable insight into various types of micro reactors.

## CH24C      PROCESS PLANT DESIGN&FLOW SHEETING TOOLS

Instruction, hours/week: 3

Credits: 3

Assessment: 40+60

### Objectives:

1. Understanding of the scope, principles, norms, accountabilities and bounds of contemporary engineering practice in the specific discipline.
2. Application of established engineering methods to complex engineering problem solving.
3. Application of systematic engineering synthesis and design processes.

**Unit-I:** Introduction: Basic concepts: General design considerations, Process design development, Layout of plant items, Flow sheets and PI diagrams, Economic aspects and Optimum design, Practical considerations in design and engineering ethics, Degrees of freedom analysis in interconnected systems, Network analysis, PERT/CPM, Direct and Indirect costs, Optimum scheduling and crashing of activities.

**Unit-II:** Hierarchy of chemical process design; Nature of process synthesis and analysis; Developing a conceptual design and flow sheet synthesis. Synthesis of reaction-separation systems; Distillation sequencing; Energy targets. Heat integration of reactors, distillation columns, evaporators and driers; Process change for improved heat integration. Heat and mass exchange networks and network design.

**Unit-III:** Flow-sheeting: Synthesis of flow sheet: Propositional logic and semantic equations, Deduction theorem, Algorithmic flow sheet generation using P-graph theory, Sequencing of operating units, Feasibility and optimization of flow sheet using various algorithms viz, Solution Structure Generation (SSG), Maximal Structure Generation (MSG), Simplex, Branch-and-bound etc.

**Unit-IV:** Analysis of Cost estimation: Factors affecting Investment and production costs, Estimation of capital investment and total product costs, Interest, Time value of money, Taxes and Fixed charges, Salvage value, Methods of calculating depreciation, Profitability, Alternative investments and replacements.

**Unit- V:** Optimum Design and Design Strategy: Break-even analysis, Optimum production rates in plant operation, Optimum batch cycle time applied to evaporator and filter press, Economic pipe diameter, Optimum insulation thickness, Optimum cooling water flow rate and optimum distillation reflux ratio.

### References:

1. Peters, M.A. and Timmerhaus, K.D., Plant Design and Economics for Chemical Engineers, McGraw Hill (2003).
2. Anil Kumar, Chemical Process Synthesis and Engineering Design, Tata McGraw Hill (1982).

3. Ulrich, G.D., A Guide to Chemical Engineering Process Design and Economics, John Wiley & Sons (1984).
4. Perry, R.H. and Green, D., Chemical Engineer's Handbook, McGraw-Hill (1997).

**Outcomes:** At the end of this course, students are able to:

1. Analyze, synthesize and design processes for manufacturing products commercially
2. Integrate and apply techniques and knowledge acquired in other courses such as thermodynamics, heat and mass transfer, fluid mechanics, instrumentation and control to design heat exchangers, plate and packed columns and engineering flow diagrams
3. Use commercial flowsheeting software to simulate processes and design process equipment
4. Recognize economic, construction, safety, operability and other design constraints
5. Estimate fixed and working capitals and operating costs for process plants