# *Master of Technology*

# *In*

# *Chemical Engineering*

## *Course Structure & Syllabus*

***Department of Chemical Engineering***

***National Institute of Technology Hamirpur***

***Hamirpur (HP) – 177005, India***

# Course Structure of M. Tech. Chemical Engineering

**SEMESTER-I**

| Sr. No. | Course No. | Course Name | Teaching Schedule | | | Hours /week | Credit |
|---|---|---|---|---|---|---|---|
| | | | L | T | P | | |
| 1 | CH-611 | Advanced Transport Phenomena | 4 | 0 | 0 | 4 | 4 |
| 2 | CH-612 | Analytical and Characterization Techniques | 4 | 0 | 0 | 4 | 4 |
| 3 | CH-613 | Mathematical Techniques | 4 | 0 | 0 | 4 | 4 |
| 4 | CH-7MN | Programme Elective-I | 4 | 0 | 0 | 4 | 4 |
| 5 | CH-7MN | Programme Elective-II | 4 | 0 | 0 | 4 | 4 |
| 6 | CH-614 | Chemical Engineering Lab. | 0 | 0 | 4 | 4 | 2 |
| | **Total** | | **20** | **0** | **4** | **24** | **22** |

**Programme Elective-I & II:** List of Programme Electives is given in the Annexure.

**SEMESTER-II**

| Sr. No. | Course No. | Course Name | Teaching Schedule | | | Hours /week | Credit |
|---|---|---|---|---|---|---|---|
| | | | L | T | P | | |
| 1 | CH-621 | Chemical Reactor Analysis and Design | 4 | 0 | 0 | 4 | 4 |
| 2 | CH-622 | Advanced Process Control | 4 | 0 | 0 | 4 | 4 |
| 3 | CH-623 | Thermodynamics of Phase and Chemical Equilibria | 4 | 0 | 0 | 4 | 4 |
| 4 | CH-7MN | Programme Elective-III | 4 | 0 | 0 | 4 | 4 |
| 5 | CH-7MN | Programme Elective-IV | 4 | 0 | 0 | 4 | 4 |
| 6 | CH-624 | Design and Simulation Lab. | 0 | 0 | 4 | 4 | 2 |
| | **Total** | | **20** | **0** | **4** | **24** | **22** |

**Programme Elective –III & IV:** List of Programme Electives is given in the Annexure.

**SEMESTER-III**

| Sr. No. | Course No. | Course Name | Hours/week | Credit |
|---|---|---|---|---|
| 1 | CH-800 | M. Tech. Dissertation | -- | 20 |
| | **Total** | | | **20** |

**SEMESTER-IV**

| Sr. No. | Course No. | Course Name | Hours/week | Credit |
|---|---|---|---|---|
| 1 | CH-800 | M. Tech. Dissertation | -- | 20 |
| | **Total** | | **--** | **20** |

# Annexure

## List of Programme Electives

**Programme Elective-I**

| | | |
|---|---|---|
| 1. | CH-711 | Novel Separation Processes |
| 2. | CH-712 | Advanced Heat and Mass Transfer |
| 3. | CH-713 | Interfacial Science and Engineering |
| 4. | CH-714 | Multiphase Flow |

**Programme Elective-II**

| | | |
|---|---|---|
| 1. | CH-716 | Bioprocess Engineering |
| 2. | CH-717 | Fuel Cell Technology |
| 3. | CH-718 | Nanoscience and Technology |
| 4. | CH-719 | Kinetics of Polymerization |

**Programme Elective-III**

| | | |
|---|---|---|
| 1. | CH-721 | Process Optimization |
| 2. | CH-722 | Process Intensification |
| 3. | CH-723 | Process Modeling and Analysis |
| 4. | CH-724 | Industrial Safety and Risk Management |

**Programme Elective-IV**

| | | |
|---|---|---|
| 1. | CH-726 | Introduction to Molecular Simulation |
| 2. | CH-727 | Introduction to Statistical Thermodynamics |
| 3. | CH-728 | Computational Fluid Dynamics |

Course Name : **Advanced Transport Phenomena**
Course Code : **CH-611**
Course Type : **Core**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To discuss the fundamentals of momentum, mass and energy balances as well as vector and tensor.
- To develop physical understanding of principles discussed and with emphasis on chemical engineering applications.
- To enable the students in advanced topics of transport phenomena fundamentals and applications to different Chemical Engineering applications.

**Course Content**

Vector and Tensors: Vector operations from a geometrical view point. Vector operation from an analytical view point, the vector differential operations, second order tensors. Various vector and tensor identities; Velocity Distributions in Laminar Flow: Shell momentum balances: Flow of a falling film, flow through a circular tube, flow through an annulus. Non- Newtonian fluids, The Equations of Change for Isothermal Systems: Equation of continuity, the equation of motion, the equation of mechanical energy. Eulerian and Lagrangian formulation. Integral form of conservation equations, Reynolds Transport theorem. Solution of unsteady flow over a wall suddenly set in motion. Flow in porous and packed bed. Creeping around sphere and cylinder; Temperature Distributions in solids and in Laminar Flow: Heat conduction with an electrical heat source, heat conduction with nuclear heat source, entropy conservation, The Equations of change for Non isothermal systems: The equations of energy, the energy equation in curvilinear coordinates, the equations of motion for forced and free convection in nonisothermal flow, use of equation of change to set up steady and unsteady heat transfer problems. Solution of unsteady heat conduction equation; Concentration Distributions in Solid and in Laminar Flow: Velocities and mass fluxes, Fick’s law of diffusion, Shell mass balances: diffusion into a falling liquid film, forced – convection mass transfer. Solution of unsteady diffusion problem; Analogies between momentum, heat and mass transfers, similitude and dimensional analysis. Interphase transport; Boundary Layer and Turbulence: Laminar boundary layer flow, heat and mass transfer. Time averaging of various conservation equations in turbulent flow, universal velocity distribution curve. Reynolds stresses and fluxes, various turbulent models.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

**CO1:** Understand the concept of vectors and tensors.
**CO2:** Understand the mechanism of momentum, heat and mass transport for steady and unsteady flow.
**CO3:** Develop analogies among momentum, energy and mass transport.
**CO4:** Solve the governing equations to obtain velocity, temperature and concentration profiles.

**Books and References**

1. Transport Phenomena by R.B. Bird, W.E. Stewart, R.N. Lightfoot, John Wiley and Sons.
2. Fundamentals of Momentum, Heat and Mass Transfer by J.R. Welty, R.E. Wilson, C.E. Wicks, John Wiley and Sons.
3. Momentum, Energy and Mass Transfer in Continua by J.C. Slattery, McGraw Hill Co.

| Course Name : **Analytical and Characterization Techniques**<br>Course Code : **CH-612**<br>Course Type : **Core** | |
|---|---|
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To impart knowledge about the statistical methods used in analyzing the data from analytical instruments.
- To introduce the fundamentals of analytical instruments used in chemical industries.
- To enable the student to identify the suitability of a particular analytical method(s) based on its merits, demerits, and limitations and to interpret the output data in required form.

**Course Content**

Introduction to Chemical Analysis: Qualitative and Quantitative analysis, fundamental theory of solution reactions i.e. chemical equilibrium, buffer solutions, Error, accuracy, precision, significant figures, correlation, regression, analysis of variance, mean and standard deviation; Spectroscopic Analysis: Introduction, theory and principles of UV-Vis Spectroscopy, Atomic Absorption Spectroscopy, Atomic Emission Spectroscopy, Mass Spectroscopy, Nuclear Magnetic Response Spectroscopy, Infrared Spectroscopy, Raman Spectroscopy; Chromatographic Analysis: Preparative, analytical chromatography, theory, principles and methodology of Thin Layer Chromatography, Liquid Chromatography (normal phase versus reversed phase chromatography), ion exchange, gel permeation and Gas Chromatography; Thermal and Electrochemical Analysis: Introduction, theory, principles and methodology of Thermo Gravimetric (TG), Differential Thermo Gravimetric (DTG), Derivative Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC)**,** theory of electrochemical anaysis, principles and methodology of Electrogravimetric analysis, Coulometry, Potentionmetry, Voltammetry; Morphology and Crystallography Analysis: Introduction, theory, principles and methodology of X-ray diffraction (XRD), scanning electron microscope (SEM), Transmission electron microscopy (TEM).

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Identify of the need of specific analytical method(s).
CO2: Describe and analyze the statistical methods.
CO3 Apply Principles of quantitative analysis used for aqueous and solid sample characterization.
CO4 Asses the specific technique employed for characterizing different solutes in water.

**Books and References**


1. Instrumental Methods of Analysis by H.H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, CBS Publisher and Distributors.
2. Thermal methods of Analysis: Principles, Application and Problems by J. Haines, Blackie Academic and Professional.
3. Chromatographic Methods by A. Braithwaite, F.J. Smith, Blackie Academic and Professional, London.
4. Principles of Instrumental Analysis by D. A. Skoog, D. M. West, F. J. Holler, T. A. Nieman, Thomson Books.
5. Instrumental Methods of Chemical Analysis, by G. R. Chatwal, S. K. Anand, Himalaya Publishing House.

Course Name : **Mathematical Techniques**
Course Code : **CH-613**
Course Type : **Core**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To introduce the student to analytical methods of solving linear algebraic equations.
- To solve ordinary differential and partial differential equations.
- To familiarize with applications of eigenvalue problems.

**Course Content**

Review of Matrix Algebra, Solvability conditions for systems of linear algebraic equations. Vector Algebra, Linear independence, Norm and Inner Product; Linear Operators, Adjoint of an operator, Self-adjoint operators. Transformations under change of basis, eigenvalues and eigenvectors, Applications to solution of systems of linear algebraic equations and systems of first order ordinary differential equations (ODEs); Second order linear ODEs, Sturm Liouville Operators, Spectral expansion, Special functions, Inverse of second order operators and Green's function; Partial differential equations (PDEs), Classification, canonical forms, Solution methods for hyperbolic, elliptic and parabolic equations, Eigen function expansion, separation of variables, transform methods, Applications from heat and mass transfer, reaction engineering; Eigenvalue Problem, Various theorems; Solution of a set of algebraic equations, Solution of a set of ordinary differential equations, Solution of a set of non-homogeneous first order ordinary differential equations (IVPs), Applications of eigenvalue problems, Stability analysis; Bifurcation theory and examples.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1 Solve linear algebraic equations.
CO2 Get knowledge of various mathematical operators.
CO3 Find solution of second order operators.
CO4 Learn solution methodology of various partial differential equations.
CO5 Apply basic knowledge of stability and bifurcation theories.

**Books and References**

1. Mathematical Methods in Chemical Engineering by S. Pushpavanam, Prentice Hall of India.
2. Applied Mathematics and Modeling for Chemical Engineers by R.G. Rice, D.D. Do, John Wiley & Sons, Inc.
3. Mathematical Method in Chemical Engineering by A. Varma, M. Morbidelli, Oxford University Press.
4. Applied Mathematical Methods for Chemical Engineers by N.W. Loney, CRC Press.
5. Numerical Methods for Engineers by S.C. Chapra, R.P. Canale, Tata McGraw-Hill, New Delhi.

| | |
|---|---|
| Course Name : **Chemical Engineering Lab.**<br>Course Code : **CH-614**<br>Course Type : **Laboratory** | |
| Contact Hours/Week: **4P** | Course Credit: **02** |

**Course Objectives**

- To impart the hands-on experience on working with various equipment and set-up.
- To verify the theoretical concepts with the help of experimental results.

**Course Content**

1. Characteristics of a fluidized bed dryer
2. Distillation in plate column
3. Membrane Separation for water purification
4. Plate type heat exchanger.
5. Determination of Effective thermal conductivity.
6. RTD study in flow reactor
7. Trickle bed reactor
8. Control of liquid level in non-interacting systems.
9. pH control in a process.
10. Pump characteristics
11. Bomb calorimeter

***Note:*** *The concerned Course Coordinator will prepare the actual list of experiments/problems at the start of semester based on above generic list.*

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Analyze characteristics of a fluidized bed dryer, distillation column and membrane process.
CO2: Evaluate the efficiency of compact heat exchangers.
CO3: Analyze RTD for flow reactors.
CO4: Design controller for a given process.
CO5: Estimate calorific value of fuel.

Course Name : **Chemical Reactor Analysis and Design**
Course Code : **CH-621**
Course Type : **Core**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To introduce the basics of heterogeneous catalytic and non-catalytic reactor design.
- To impart the characteristics of non-ideal reactors by RTD analysis.
- To introduce the concept of multiphase reactors.

**Course Content**

Review of design of ideal isothermal homogeneous reactors for single and multiple reactions; Residence time distribution (RTD) of ideal reactors, interpretation of RTD data, flow models for non-ideal reactors – axial dispersion, N-tanks in series, and multiparameter models, diagnostics and troubleshooting, influence of RTD and micromixing on conversion; Adiabatic and non-adiabatic operations in batch and flow reactors, optimal temperature progression, hot spot in tubular reactor, autothermal operation and steady state multiplicity in continuously stirred tank reactor (CSTR) and tubular reactors; Introduction to multiphase catalytic reactors, effectiveness factor, selectivity, catalyst deactivation, use of pseudo-homogeneous models for design of heterogeneous catalytic reactors (fixed and fluidized beds); Gas-liquid-solid reactors, hydrodynamics and design of bubble column, slurry and trickle-bed reactors. Introduction to laboratory reactors.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Gain through knowledge on catalyst physical properties and catalyst characterization
CO2: Awareness on kinetics of catalytic and non-catalytic chemical reaction,
CO3: Get knowledge about multiphase reactors
CO4: Familiarize with the design of catalytic and non-catalytic reactor

**Books and References**

1. Chemical Reaction Engineering by O. Levenspiel, Wiley Eastern, New York.
2. Chemical Engineering Kinetics by J.M. Smith, McGraw Hill, New York.
3. Elements of Chemical Reaction Engineering by H.S. Fogler, Prentice Hall of India Ltd.
4. Chemical Reactor Analysis and Design by G.F. Froment, K.B Bischoff, John Wiley & Sons, New York.
5. Heterogeneous Reactions Analysis Vol. 1: Gas-Solid and Solid-Solid Reactions by L.K. Doraiswamy, M.M. Sharma, Wiley.

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|---|---|
| Course Name : **Advanced Process Control**<br>Course Code : **CH-622**<br>Course Type : **Core** | |
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To impart knowledge about the advanced control methods used in industries and research.
- To understand the stability of multi-variable control system.
- To enable the students to understand the various factors that affects the control system.

**Course Content**

Review of Systems: Review of first and higher order systems, closed and open loop response. Response to step, impulse and sinusoidal disturbances. Transient response. Block diagrams; Feed Back Control: stability using root-locus, and frequency response method, time-integral performance criteria of controllers and tuning methods; Advanced Control Systems: Control of systems with inverse response, dead time compensator, cascade control, selective control, split-range control, feed forward and ratio control, internal model, adaptive and inferential control; Multivariable Control Systems: Alternative control configurations, interaction and decoupling of loops, relative gain-array method, control for complete plants, State Space Methods: State variables, description of physical systems, transition and transfer function matrices, use in multivariable control for interacting systems; Digital Control Systems: Review of Z transform, elements of digital control loop, sampling and reconstruction of signals, conversion of continuous to discrete-time models, discrete time response and stability, design of controllers, control algorithms.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

**CO1:** Perform stability analysis and controller tuning
**CO2:** Select and design advanced controllers that need to be used for specific problems
**CO3:** Design controllers for interacting multivariable systems
**CO4:** Understand the dynamic behavior of discrete time processes and design discrete controllers

**Books and References**


1. Process System Analysis and Control by D.R. Coughanowr, S. LeBlanc, McGraw Hill.
2. Chemical Process Control – An Introduction to Theory and Practice by G. Stephanopoulos, Prentice-Hall of India.
3. Process Dynamics Control by D.E. Seborg, T.F. Edgar, D.A. Mellichamp, John Wiley & Sons.
4. Process Control: Modeling, Design and Simulation by B.W. Bequette, Prentice Hall of India.
5. Process Dynamics Modeling and Control by B.A. Ogunnaike, W.H. Ray, Oxford University Press.

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|---|---|
| Course Name : **Thermodynamics of Phase and Chemical Equilibria**<br>Course Code : **CH-623**<br>Course Type : **Core** | |
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To impart knowledge about the basic concepts of chemical engineering thermodynamics.
- To introduce the fundamental concepts relavent to different chemical process.
- To enable the students to understand the factors that causes the thermodynamic challenges in different chemical industries.

**Course Content**

Review of fundamental principles: Review of thermodynamic laws, thermodynamic potentials, thermodynamic stability, and thermodynamic properties of pure substances; Thermodynamic properties of mixtures: Ideal gas mixtures, ideal or Lewis mixtures chemical potential and fugacity, partial molar properties, calculation of fugacity and fugacity coefficients, excess properties, concept of activity coefficient, correlative activity coefficient models; Phase equilibria: Fundamental VLE equation,VLE at low, moderate and high pressures, azeotropic data, multi-component VLE, thermodynamic consistency test of VLE data, liquid-liquid equilibria, chemical reaction equilibria; Intermolecular forces: Interactions between molecules, electrostatics and dipoles, potential energy functions, molecular dynamics simulations; Statistical thermodynamics: Quantum mechanical aspects, thermodynamic probability and entropy, Boltzmann's distribution law, partition function, thermodynamic properties in terms of partition functions, partition functions of polyatomic molecules.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Identify and understand the peculiar thermodynamic properties.
CO2: Describe the different thermodynamic aspects based on fundamental concepts.
CO3: Apply principle of thermodynamics laws to determine the different equilibrium states.
CO4: Assess the importance of applications of thermodynamic laws in related fields.

**Books and References**


1. Molecular Thermodynamics of Fluid Phase Equilibria by J. M. Prausnitz, R. N. Lichtenthaler, E. Gomes-de-Azevedo, Prentice Hall.
2. Chemical, Biochemical and Engineering Thermodynamics by S.I. Sandler, John Wiley & Sons.
3. Chemical Engineering Thermodynamics by Y. V. C. Rao, Universities Press.
4. Introduction to Chemical Engineering Thermodynamics by J. M. Smith, H. C. Van-Ness, M. M. Abbott, McGraw Hill.
5. Engineering and Chemical Thermodynamics by M. D. Koretsky, Wiley.

| | |
|---|---|
| Course Name: **Design and Simulation Lab.**<br>Course Code: **CH-624** | |
| Contact Hours/Week: **4P** | Course Credit: **02** |

**Course Objectives**

- To impart the hands-on experience on working with various equipment and set-up.
- To verify the theoretical concepts with the help of experimental results.

**Course Content**

1. Problems on heat exchanger design.
2. Problems on distillation column design.
3. Problems on reactor design.
4. Pressure drop in piping network.
5. Heat and mass transfer around bluff bodies.
6. Design and fluid flow in micro-channels.
7. Heat transfer through composite solid bodies.
8. Solution of ordinary differential equations.
9. Solution of partial differential equations.
10. Solution of coupled partial differential equations.

***Note:*** *The concerned Course Coordinator will prepare the actual list of experiments/problems at the start of semester based on above generic list.*

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Design and simulate mixer, splitter, heat exchangers, reactors, distillation columns etc.
CO2: Learn computational methods required in industry and research.
CO3: Gain knowledge about several design software.
CO4: Analyze the simulated results.

Course Name : **Novel Separation Processes**
Course Code : **CH-711**
Course Type : **Programme Elective-I**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To learn the principle and technical concepts of rate governed separation processes.
- To understand the industrial applications of various separation process.
- To apply the knowledge in designing process equipment.

**Course Content**

Introduction: Separation processes in chemical and biochemical industries, categorization of separation processes, separation factor, equilibrium and rate governed processes; Membrane Separation: Membrane materials, Polymeric membranes, Asymmetric and symmetric membranes, Perm-selectivity, Physical factors in membrane separation, Pore size, osmotic pressure, partition coefficient and permeability; Transport through porous membranes- bulk flow, gas diffusion, Knudsen diffusion, liquid diffusion; Transport through nonporous membranes, solution diffusion for liquid mixtures, solution diffusion for gas mixtures, membrane separation factor, ideal membrane separation factor, external mass transfer resistances, concentration polarization and fouling; Membrane separation processes: Reverse osmosis, Ultrafiltration, Nano filtration, Gas permeation, pervaporation, Liquid membrane separation. Dialysis, electro-dialysis; Sorption Separation: Principles of Chromatography and Ion exchange, Types of chromatographic techniques, Retention theory for calculation of Partition coefficient, Band broadening and its factors, Column Chromatography for gas and liquid mixtures separation, Detectors, Design controlling factors, Ion exchangers, equipments, Ion exchange equilibria, Kinetics and mass transport mechanism, regeneration; Other separation processes: Micellar enhanced separation processes, Cloud point extraction, electrophoresis, Supercritical fluid extraction.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Get knowledge about the about various advancements in separation processes.
CO2: Understand the mechanism membrane separation process and their applications.
CO3: Analyze and design membranes in industrial applications.
CO4: Have knowledge about chromatographic techniques.

**Books and References**


1. Handbook of Separation Process Technology by R.W. Rousseau, John Wiley & Sons, New York.
2. Large Scale Adsorption & Chromatography by W.C. Wankat, CRC Press Inc.
3. Advanced Membrane Technology and Applications by N.N. Li, A.G. Fane, H.W.S. Winston, T. Matsuura (Eds.), John Wiley & Sons, Inc.
4. Separation Processes by C.J. King, Tata McGraw Hill.
5. Separation process Principles by J.D. Seader, E.J. Henley, D.K. Roper, John Wiley & Sons.

| | |
|---|---|
| Course Name : **Advanced Heat and Mass Transfer**<br>Course Code : **CH-712**<br>Course Type : **Programme Elective-I** | |
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To impart the knowledge of steady state and unsteady state heat conduction in various geometry.
- To train students on multicomponent mass transfer and mass transfer accompanied by irreversible and reversible reactions.
- To enable the students to design heat and mass transfer equipment.

**Course Content**

Steady state heat conduction: Review of heat transfer basic laws, General conduction equation, side conditions. One dimensional heat conduction without generation, Plane slab, Circular cylindrical shell, Spherical shell, Variable thermal conductivity, Conduction across composite barriers, Critical insulation thickness; Unsteady state condition: Exact analytical solutions and charts for infinite slab, cylinder and sphere, Semi-infinite slab, Lumped parameter method of transient analysis, Heat exchanger design: Process design of compact heat exchangers, condensers; Mass transfer: Review of mass transfer, Basic laws, Mass transfer theories, Dimensionless numbers, Multicomponent distillation: Degree of freedom analysis, Key components, Column operating conditions, Fenske and Underwood equation, cascade processes calculations, Lewis-Matheson method, Thiele-Geddes method, Matrix methods, Rate based method to design a packed column, Pressure swing and azeotropic distillation, Modeling and simulation of absorption; Transient Diffusion and Mass Transfer with Chemical Reaction: Transient diffusion in 3D and its solution, determination of diffusivity, Diffusion with reaction, Film, penetration and surface renewal theory with reaction, irreversible second order reaction, instantaneous reaction.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Derive the governing differential equation for conduction and convection heat transfer.
CO2: Solve the differential equation to obtain temperature profile in solid or fluid.
CO3: Solve the problems on multicomponent mass transfer and mass transfer with chemical reaction.
CO4: Design heat and mass transfer equipment.

**Books and References**


1. Heat Transfer by J. Sucec, Jaico Publishing House.
2. Heat Transfer by J.P. Holman, P. R. S. White, McGraw Hill.
3. Heat Transfer: Principles and Applications by B. K. Dutta, Prentice Hall of India, New Delhi.
4. Separation Processes and Principles by J. D. Seader, E. J. Henly, John Willey.
5. Multicomponent Mass Transfer by R. Taylor, R. Krishna, John Wiley.
6. Principles of Mass Transfer and Separation Processes by B. K. Dutta, Prentice Hall of India, New Delhi.

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|---|---|
| Course Name : **Interfacial Science and Engineering**<br>Course Code : **CH-713**<br>Course Type : **Programme Elective-I** | |
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To discuss the basic concepts of colloids, surface and interfacial energies and tensions, intermolecular and surface forces, stability of colloids.
- To enable the students to solve the problems effectively in the field of Chemical Engineering, Analytical and Physical Chemistry, Biochemistry and Environmental Science, Materials Science, Petroleum Engineering and Nanotechnology.

**Course Content**

Basic concepts of colloids and interfaces: Introduction; Examples of interfacial phenomenon, Solid fluid interfaces, Colloids: colloids and interfaces, Classification of colloids, Electric charge on colloidal particles, Stability of colloids– kinetic and thermodynamic stabilities, Preparation of colloids, Parameters of colloidal dispersions; Properties of colloidal dispersions: Sedimentation under gravity and in a centrifugal field, Brownian motion, Osmotic pressure, Optical properties - light scattering, TEM, SEM, DLS, SANS, Electrical properties: reciprocal relationship and Zeta-potential. Properties of lyophilic sols. Rheological properties of colloidal dispersions – Einstein's equation of viscosity, Mark-Houwink equation of polymer solutions; Surfactants and their properties: Surfactants and their properties: anionic surfactants, cationic surfactants, Zwitterionic surfactants, nonionic surfactants, Gemini surfactants and biosurfactants, HLB, Liquid crystals, Micellisation of solutions, thermodynamics of micellisation, Kraft point and cloud points, Emulsions and Microemulsions, Foams; Surface and interfacial tensions: Surface tension, Interfacial tension, Contact angle and wetting, Shape of surfaces and interfaces, Measurement of surface and interfacial tension, Measurement of contact angle; Intermolecular and surface forces: Van der walls forces, Electrostatic double layer force, DLVO theory, Kinetics of coagulation, Characterization of solid surfaces: Applications in detergents, personalcare products, pharmaceuticals, nanotechnology, food, textile, paint and petroleum industries.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

**CO1:** Understand the basics properties of the colloidal material and forces governing them.
**CO2:** Understand the particle aggregation behavior in aqueous and organic dispersions.
**CO3:** Design a colloidal dispersion having long-term stability.
**CO4:** Prepare emulsions and microemulsions with the use of surfactants and polymers.

**Books and References**


1. Principles of Colloid and Surface Chemistry by P. C. Hiemenz, R. Rajagopalan, Marcel Dekker, New York.
2. An Introduction to Interfaces and Colloids: The Bridge to Nanoscience by J. C. Berg, World Scientific, Singapore.
3. Intermolecular and Surface Forces by J. N. Israelachvili, Academic Press, Elsevier.
4. Physical Chemistry of Surfaces by A. W. Adamson, A. P. Gast, John Wiley & Sons, New York.
5. Interfaces and Colloids: Principles and Applications by D. Myers, John Wiley & Sons.
6. Foundations of Colloid Science by R. J. Hunter, Oxford University Press, New York.
7. Colloidal Dispersions by W. B. Russel, D. A. Saville, W. R. Schowalter, Cambridge University Press.

Course Name : **Multiphase Flow**
Course Code : **CH-714**
Course Type : **Programme Elective-I**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To introduce a general introduction to the underlying concepts of multiphase flows and different approaches to model such flows under different conditions.
- To impart the knowledge about the real life examples and their importance in process industries with multiphase contactors.

**Course Content**

Introduction to multiphase flow, types and applications, Common terminologies, flow patterns-identification and classification - flow pattern maps and transition, momentum and energy balance - homogeneous and separated flow models -correlations for use with homogeneous and separated flow models.

Measurement Techniques for experimental flow, one dimensional steady homogenous flow, Analysis of concept of choking and cavitation

One dimensional steady separated flow model, Application of separated model for flow with phase change. Application of separated model in analysis of annular and stratified flow

General theory of drift flux model. Application of drift flux model to bubbly and slug flow, Modification of Drift flux model for liquid-liquid and gas-liquid flows in mini channels

Introduction to three phase flow, Dynamics of gas-solid liquid contactors (agitated vessels, packed bed, fluidized bed, pneumatic conveying, bubble column, trickle beds), applications, flow regime identification, pressure drop and volume fraction estimation techniques.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Analyze, characterize the multiphase systems and appreciate the role of structure in multiphase flows and the role it plays in obtaining engineering solutions.

CO2: Understand the assumptions may be made to simplify multiphase flows and when they might be employed.

CO3: Understand the limitations of modeling multiphase flows.

CO4: Solve engineering problems involving multiphase flows.

**Books and References**

1. One dimensional Two Phase Flow by G. B. Wallis, McGraw-Hill, New York.
2. Measurement of Two Phase Flow Parameters by G. F. Hewitt, Academic Press, New York.
3. Two-Phase flow, Boiling, and Condensation in conventional and Miniature Systems by S.M. Ghiaasiaan, Cambridge University Press.
4. Fundamentals of Multiphase Flow by C. E. Brennen, Cambridge University Press.
5. Two Phase Flow and Heat Transfer by D. Butterworth, G. F. Hewitt (Edited), Oxford University Press.
6. Convective Boiling and Condensation by J. G. Collier, J. R. Thome, Oxford University Press.

| Course Name : **Bioprocess Engineering**<br>Course Code : **CH-716**<br>Course Type : **Programme Elective-II** | |
|---|---|
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To understand the principles and stoichiometry of biological processes.
- To understand the kinetics, modeling and design of biochemical processes.
- To explain various industrial relevant biochemical processes.

**Course Content**

Introduction: Biotechnology, Biochemical Engineering, Biological Process, Definition of Fermentation, Cell theory, structure of microbial cells, classification of microorganism, Enzyme assay, Sterilization and pasteurization, batch and continuous sterilization of media, plate and direct injection sterilization; Thermal death kinetics of spores, cells and viruses; Enzyme & Cell Kinetics: Introduction, Simple Enzyme Kinetics, Enzyme Reactor with Simple Kinetics, Inhibition of Enzyme Reactions, Other influences on Enzyme Reactions, Experiment: Enzyme Kinetics, Growth Cycle for Batch Cultivation, Enzyme immobilization; Bioreactor design: Design of batch and continuous fermentations with and without recycles, bioreactors in series, product synthesis kinetics, over all kinetics, thermal death kinetics of spores and cells, transient growth kinetics, deviation from Monod model; Transport Processes: Gas-liquid mass transfer, oxygenation of fermentation broth; bubble and mechanical aeration and agitation, design and power requirement of gassed and un-gassed systems for various impellers, hold-up; Aerobic and Anaerobic Fermentations: Design and analysis of typical aerobic and anaerobic fermentation processes, manufacture of antibiotics, alcohol and other fermentation products, Downstream processing: Strategies to recover and purify Products, Separation of insoluble Products, Cell disruption, Separation of soluble products, finishing steps for purification.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Gain general knowledge about cell cultivation and enzymatic processes.
CO2: Understand enzyme kinetics and cell kinetics.
CO3: Design various bioreactors.
CO4: Get the knowledge about downstream processing.

**Books and References**


1. Biochemical Engineering Fundamentals by J. E. Bailey, D. F. Olis, McGraw-Hill.
2. Biochemical Engineering by M. Doble, S. N. Gummadi, Prentice Hall.
3. Bioprocess Engineering by M. L. Schuler, F. Kargi, Prentice Hall.
4. Chemical Engineering Vol -3 by J. M. Coulson, R. E. Richardson, Elsevier.

Course Name : **Fuel Cell Technology**
Course Code : **CH-717**
Course Type : **Programme Elective-II**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To understand about basics of fuel cells and their working principle.
- To impart the knowledge of various types of fuel cells and their applications.
- To design and analysis the performance of fuel cell.

**Course Content**

Basic Electrochemistry, Overview of fuel cells: Low and high temperature fuel cells; Fuel cell thermodynamics - heat, work potentials, prediction of reversible voltage, fuel cell efficiency; Fuel cell reaction kinetics - electrode kinetics, overvoltages, Tafel equation, charge transfer reaction, exchange currents, electrocatalysis, simplified activation kinetics, catalyst-electrode design, Fuel cell charge and mass transport - flow field, transport in electrode and electrolyte; Fuel cell characterization: in-situ and ex-situ characterization techniques, I-V curve, frequency response analyses; Fuel cell system integration; PEM Fuel Cell components: Anode and Cathode materials, catalysts, membrane, Fuels for fuel cells- PEM Fuel cell stacks - Rate of mass transfer of reactants and products - water management – current collections and gas removal- Bipolar plates- flow distribution – Heat and water removal from the stack; Balance of plant; Hydrogen production from renewable sources and storage; safety and norm issues, cost expectation and life cycle analysis of fuel cells.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Learn basics and working principles of the Fuel cell technology.
CO2: Select the suitable materials for electrode, catalyst, membrane for the fuel cells.
CO3: Understand the pressure drop and velocity distribution in single cell as well as stack.
CO4: Design and stack making process for real field applications.

**Books and References**

1. Fuel Cell Fundamentals by R.P. O'Hayre, S. Cha, W. Colella, F. B. Prinz, John Wiley & Sons, Inc.
2. Electrochemical Methods by A.J. L. R. Bard, Faulkner, John Wiley & Sons, Inc.
3. Fuel Cell Science and Technology by S. Basu, (Edited), Springer.
4. Principles of Fuel Cells by H. Liu, Taylor & Francis.

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| Course Name : **Nanoscience and Technology**<br>Course Code : **CH-718**<br>Course Type : **Programme Elective-II** | |
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To impart knowledge about the basic concepts of nanomaterials and nanotechnology.
- To introduce the fundamental concepts relevant to different classes of nanomaterials.
- To enable the students to understand the various characterization techniques of nanoparticles.

**Course Content**

Introduction: Definition of Nano, Scientific revolution-Atomic Structure and atomic size, emergence and challenges of nanoscience and nanotechnology, carbon age-new form of carbon (CNT to Graphene), influence of nano over micro/macro, size effects and crystals, large surface to volume ration, surface effects on the properties; Structure and properties of nanomaterials: One dimensional, Two dimensional and Three dimensional nanostructured materials, Quantum Dots shell structures, metal oxides, semiconductors, composites, mechanical-physical-chemical properties; Synthesis Methods: Top-down approach, bottom-up approach, grinding, planetary milling and comparison of particles sol-gel methods, sonochemical approach, physical vapor deposition, chemical vapor deposition, wet deposition techniques, self-assembly, supramolecular approach, molecular design and modeling; Characterization and Fabrication Techniques: TEM, SEM and AFM technique, Fluorescence Microscopy and Imaging, scanning and tunneling microscopy, Nanolithography, Thin film processes, semiconductors, MEMS: Overview and history of development, Dip Pen Lithography; Application of Nanomaterial: Ferroelectric materials, coating, molecular electronics and nanoelectronics, biological and environmental, membrane based application, polymer based application.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Identify and understand the peculiar properties of materials at nanoscale.
CO2: Describe the chemistry involved in the synthesis of nano-materials.
CO3: Apply principle of nanotechnology to understand the properties of nano-materials.
CO4: Assess the important applications of nano-materials in related fields.

**Books and References**


1. Introduction to Nanoscience and Nanotechnology by G.L. Hornyak, H.F. Tibbals, J. Dutta, J.J. Moore, CRC Press.
2. Introduction to Nanotechnology by C.P. Poole, F.J. Owens, Wiley.
3. Nanotechnology by M. Ratner, D. Ratne, Prentice Hall.
4. Nanotechnology: Basic Science and Emerging Technologies by M. Wilson, K. Kannagara, G. Smith, M. Simmons, B. Raguse, CRC Press, Boca Raton.
5. Nanotechnology: Science, Innovation, and Opportunity by L.E. Foster, Prentice Hall.

Course Name : **Kinetics of Polymerization**
Course Code : **CH-719**
Course Type : **Programme Elective-II**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To discuss about the basics of polymer and their classification properties, synthesis methods.
- To impart the knowledge about detailed kinetics of various polymerization techniques.

**Course Content**

Introduction & classification: polymer, monomer, average chain length and molecular weight of polymers, classification based on (i) origin (natural, synthetic and semi-synthetic) (ii) application and physical properties (resin, plastic, rubber, fiber) (iii) Thermal response (Thermoplastics and thermosetting), (iv) line structure (branched, crosslinked and linear polymer), (v) Tacticity (atactic, synditactic and isotactic) (vi) polarity (polar and non-polar) and (vii) crystallinity (amorphous, crystalline and semi-crystalline), (viii) Polymerization processes (addition and condensation polymerization); Addition polymerization: free radical, anioic and cationic polymerization, overall scheme, rate expression for cationic and anionic polymerization, Kinetics and mechanism of free radical polymerization: overall scheme, rate expression for radical polymerization, integrated rate of polymerization expression, methods of initiation: thermal decomposition, redox initiation, photochemical initiation, dead-end polymerization, chain length and degree of polymerization, kinetic chain length, chain transfer, deviation from ideal kinetics, autoacceleration, polymerization-depolyerization equilibrium; Techniques of polymerization: bulk, solution, suspension and emulsion polymerization, kinetics of emulsion polymerization, Kinetics of Copolymerization by radical chain polymerization: binary copolymer equation, types of copolymers, integrated binary copolymer equation, Kinetics of ionic polymerization: anionic, cationic and coordination polymerization; Kinetics of condensation polymerization: reactivity of functional groups, average functionality, Rate expression for condensation polymerization- catalyzed and non-catalyzed, equilibrium considerations- closed and open drive system, control of molecular weight, branching and crosslinking.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Get the knowledge of various types of polymers.
CO2: Estimate various types of molecular weight of polymers.
CO3: Understand the mechanism of various types of polymerization.
CO4: Derive the kinetic expression for various types of polymerization techniques.

**Books and References**

1. Polymer Science and Technology: Plastics, Rubber, Blends and Composites by P. Ghosh, Tata McGraw Hill.
2. Advanced Polymer Chemistry: A Problem Solving Guide by M. Chanda, Marcel Dekker.
3. Polymer Chemistry by C.E. Carraher, CRC Press.
4. Polymer Science by V.R. Gowarikar, N.V. Vishwanathan, J. Sreedhar, New Age International.
5. Fundamentals of Polymer Engineering by R.K. Gupta, A. Kumar, Marcel Dekkar.

Course Name : **Process Optimization**
Course Code : **CH-721**
Course Type : **Programme Elective-III**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To understand the concepts and origin of the different optimization methods.
- To get a broad picture about various applications of optimization in Chemical Engineering.
- To discuss about the various emerging optimization techniques used in industry and research.

**Course Content**

Introduction: Optimization and calculus based classical optimization techniques, One Dimensional Minimization Methods: Elimination methods- equally spaced points method, Fibonacci method and golden section method; Interpolation methods- quadratic interpolation and cubic interpolation, Newton and quasi-Newton methods; Linear Programming: Graphical representation, simplex and revised simplex methods, duality and transportation problems; Multivariable Non-Linear Programming: Unconstrained- univariate method, Powell’s method, simplex method, rotating coordinate method, steepest descent method, Fletcher Reeves method, Newton’s method, Marquardt’s method and variable metric (DFP and BFGS) methods; Constrained- complex method, feasible directions method, GRG method, penalty function methods and augmented Lagrange multiplier method; Dynamic Programming: Multistage processes- acyclic and cyclic, suboptimization, principle of optimality and applications; Geometric Programming (GP): Differential calculus and Arithmetic-Geometric inequality approach to unconstrained GP; Constrained GP minimization; GP with mixed inequality constraints and Complementary GP, Emerging Optimization Techniques: Genetic algorithm, simulated annealing, particle swarm and ant colony optimization.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Formulate objective function for a given problem
CO2: Understand unconstrained single variable optimization and unconstrained multi variable optimization
CO3: Understand linear programming and nonlinear programming techniques
CO4: Use dynamic programming and semi definite programming for optimization

**Books and References**


1. Optimization of Chemical Processes by T.F. Edgar, D.M. Himmelblau, L.S. Lasdon, McGraw Hill.
2. Optimization: Theory and Practice by G.S.G. Beveridge, R.S. Schechter, McGraw Hill.
3. Engineering Optimization Theory and Practice by S.S. Rao, Wiley.
4. Optimization for Engineering Design: Algorithms and Examples by K. Deb, Prentice Hall of India.

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| Course Name : **Process Intensification**<br>Course Code : **CH-722**<br>Course Type : **Programme Elective-III** | |
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To impart knowledge about the energy and mass targets in design of processes.
- To introduce the fundamental Process Heat Exchange Networking.
- To enable the students to identify the energy minimization in process industries.

**Course Content**

Introduction: Process Intensification (PI) and its building blocks, available techniques for implementation of PI, application of PI; Pinch Technology: Basic concepts, role of thermodynamics. Data extraction, targeting, designing, optimization-supertargeting. Grid diagram, composite curve, problem table algorithm, grand composite curve; Targeting of Heat Exchanger Network (HEN): Energy targeting, area targeting, number of units targeting, shell targeting, cost targeting, Design of HEN: Pinch design methods, heuristic rules, stream splitting, design for maximum energy recovery (MER), multiple utilities and pinches, threshold problem, loops and paths, non-MER design, remaining problem analysis, driving force plot; Heat Integration of Equipment: Heat engine, heat pump, distillation column, reactor, evaporator, drier, refrigeration system; Reactive and hybrid separations: Concept of reactive separations, reactive distillation, membrane-based reactive separation, reactive crystallization, hybrid separations, extractive distillation, adsorptive distillation, membrane distillation, design applications, Industrial practice: Methodology and applications, commercial examples of process intensification.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Identify the fundamentals of process integration
CO2: Describe the analysis and design of heat exchanger networks for minimization of annual costs
CO3: Apply the principles of pinch analysis on various chemical engineering process equipment.
CO4: Assess the strategies for retrofitting existing process plant, integration of energy demands of multiple processes to minimize the water consumption and waste generation.

**Books and References**


1. Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy by I.C. Kemp, Butterworth Heinemann.
2. Chemical Process Design and Integration by R. Smith, Wiley.
3. Heat Exchanger Network Synthesis by U.V. Shenoy, Gulf Publishing.
4. Handbook of Process Integration (PI): Minimisation of Energy and Water Use, Waste and Emissions by J. Klemes (Edited), Woodhead Publishing.
5. Process Intensification in Practice by C-d. Weerd, John Wiley and Sons.
6. Re-engineering the Chemical Processing Plant: Process Intensification by A. Stankiewicz, J.A. Moulijn, Marcel Dekker Inc.

Course Name : **Process Modeling and Analysis**
Course Code : **CH-723**
Course Type : **Programme Elective-III**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To introduce basic concepts and types of models.
- To develop mathematical models of chemical engineering systems and their simulation.
- To enable the students to develop models for discrete systems.

**Course Content**

Introduction to modeling, a systematic approach to model building, classification of models, Development of steady state and dynamic lumped and distributed parameter models based on conservation principles. The transport phenomena models: Momentum, energy and mass transport models. Analysis of ill-conditioned systems; Classification of systems, system's abstraction and modeling, 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: Series of isothermal constant holdup CSTRs, CSTRs with variable holdups, Non-isothermal CSTR, Batch reactor, Batch distillation with holdup, Ideal binary distillation column, Lumped parameter model of gas absorber, Model for heat exchanger, Model for interacting & non-interacting tanks; Discrete systems: difference equations, state-transition diagrams, cohort simulation of Markov models, random processes, descriptive statistics, hypothesis testing, probabilistic distributions, pseudo-random numbers, Monte Carlo methods, numerical simulation of continuous-time dynamics, discrete-event systems, cellular automata, Moore machines, real-world system examples: Chemical Systems.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Understand model building techniques.
CO2: Develop first principles, grey box and empirical models for systems.
CO3: Develop mathematical models for engineering processes.
CO4: Model discrete time systems.

**Books and References**


1. Process Modeling and Simulation in Chemical, Biochemical and Environmental Engineering by A.K. Verma, CRC Press.
2. Chemical Process Modeling and Computer Simulation by A.K. Jana, Prentice Hall.
3. Mathematical Modeling: Case Studies by J. Caldwell, K.S.N. Douglas, Kluwer Academic Publishers.
4. Conservation Equations and Modeling of Chemical and Biochemical Processes by S.S.E.H. Elnashaie, P. Garhyan, Marcel Dekker Publishers.
5. Process Modelling and Model Analysis by K.M. Hangos, I.T. Cameron, Academic Press.
6. Chemical Engineering Dynamics by J. Ingham, I.J. Dunn, E. Heinzle, J.E. Prenosil, J.B. Snape, Wiley.

Course Name : **Industrial Safety and Risk Management**
Course Code : **CH-724**
Course Type : **Programme Elective-III**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To impart deeper understanding at the principles of industrial safety and procedures to be followed in chemical industries.
- To discuss about the hygiene and occupational diseases and their control.
- To enable the students to understand risk management.

**Course Content**

Industrial Hazards: Chemical hazards classification, Radiation hazards and control of exposure to radiation, Fire hazards, Types of fire and prevention methods, Mechanical hazards, Electrical hazards, Construction hazards; Psychology and Hygiene: Industrial psychology, Industrial hygiene, Nature and types of work places, Housekeeping, site selection and plant layout, Industrial lighting and ventilation, Industrial noise; Occupational diseases and safety control: Occupational diseases and prevention methods, Instrumentation and control for safe operation, Pressure, Temperature and Level controllers, Personal protective equipments; Risk Management and Analysis: Safety organization, safety education and training, steps in Risk management, Safety analysis, Case studies pertaining to chemical industries; Legislations and economics: Factory Act. ESI Act, Environmental Act. Workmen - compensation Act, Provisions under various acts, Economics of safety. Financial costs to individual, family, organization and society, Budgeting for safety.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Know about accident prevention and hazard analysis techniques.
CO2: Identify the process safety responsibilities.
CO3: Understand the psychological approach to process safety.
CO4: Learn the legislations pertaining to safety in chemical industries.

**Books and References**


1. Lees' Loss Prevention in the Process Industries: Hazard Identification, Assessment and Control by F.P. Lees, Butterworth-Heinemann.
2. Safety and Accident Prevention in Chemical Operation by H.H. Fawcett, W.S. Wood, Wiley Inter-Science.
3. Guide for Safety in the Chemical laboratory by Manufacturing Chemists Association, Van Nostrand Reinhold Company, New York.
4. Industrial Safety and Laws 1993 by Indian School of Labour Education, Madras.
5. Chemical Process Safety, Fundamentals with Applications by D.A. Crowl, J.F. Louvar, Prentice Hall.

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| Course Name : **Introduction to Molecular Simulation**<br>Course Code : **CH-726**<br>Course Type : **Programme Elective-IV** | |
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To impart knowledge about the basic concepts of molecular simulation.
- To introduce the fundamental concepts relevant to different computational techniques.
- To enable the students to understand the factors those cause the computation of different thermodynamic properties.

**Course Content**

Concepts of Statistical Mechanics: Molecular Mechanics, Statistical Ensemble, Phase Space, Thermodynamic Limit, Trajectory, atomic and molecular interaction; Entropy and equation of State: Definition of Entropy, Ideal Gas Entropy, Mechanical and Chemical Coupling, Fundamental Equation of State, Ideal Gas Law, Virial Equation of State; Partition functions and ensembles: Partition function, Micro-caninical ensemble, canonical ensemble, Boltzmann distribution; Short range Interactions: Repulsive Interaction, Dispersive Interaction, Lennard-Jones Potential, Unlike Interaction, Long range Interactions: Electrostatic Interactions, Force Field Design, Separation of Scales; Molecular Simulation Algorithms: Molecular Dynamics, Thermostat and Barostat, Monte Carlo Method, Metropolis Algorithm

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Identify and understand the peculiar molecular simulation techniques.
CO2: Describe the different simulation techniques to compute the entropy, Gibbs and Helmohltz free energy, etc.
CO3: Apply principles to compute the different thermodynamic properties.
CO4: Assess the importance of applications of molecular simulation techniques in related fields.

**Books and References**


1. Computer Simulation of Liquids by M. P. Allen, D. J. Tildesley, Clarendon Press.
2. Understanding Molecular Simulation: From Algorithm to Application by D. Frenkel, B. Smit, Academic Press.
3. Physical Chemistry, a Molecular Approach by D. McQuarrie, J. D. Simons, University Science Books.
4. Introduction to Modern Statistical Mechanics by D. Chandler, Oxford University Press.
5. Introduction to Statistical Thermodynamics by T. L. Hill, Addison-Wesley.

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| Course Name : **Introduction to Statistical Thermodynamics**<br>Course Code : **CH-727**<br>Course Type : **Programme Elective-IV** | |
| Contact Hours/Week: **4L** | Course Credit: **04** |

**Course Objectives**

- To impart knowledge about the basic concepts of statistical thermodynamics.
- To introduce the fundamental concepts relevant to entropy, Gibbs and Helmohltz free energy, etc.
- To enable the students to understand the factors that causes the thermodynamic issues in any chemical process by different computational techniques.

**Course Content**

Introduction: Elementary statistical mechanics, postulates of statistical mechanics, quantum mechanical aspects, Boltzmann's distribution law, isolated system, entropy, microscopic and macroscopic properties, microscopic and macroscopic descriptions of the state of a system; Partition functions and probability: Partition functions, derivatives and thermodynamic properties, system of independent particles, compressibility equation, thermodynamic probability, probability distribution. Ensembles Averages: Canonical, microcanonical, and grand canonical ensemble, NVE, NVT, NPT, μVT, Equivalence of ensembles; Fluctuations and equilibration: Fluctuation, energy, density, pressure, entropy maximization, configurational integral, Virial equation of state, ideal and non-ideal monoatomic and polyatomic gases, particle densities, thermal equilibrium, chemical equilibrium in ideal gas mixtures; Distribution functions: Distribution functions theories, perturbation theories, molecular distribution functions, density expansion of pair correlation function, direct correlation function, lattice models, average energy, compressibility; Applications through simulations: Thermo-physical property calculations, study of phase equilibria, Gibbs ensemble, thermodynamic integration, free energy evaluation by molecular simulation techniques, surface adsorption, adsorption isotherms, molecular interaction.

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Identify and understand the peculiar thermodynamic properties.
CO2: Describe the different computational techniques to compute entropy, Gibbs and Helmohltz free energy, etc.
CO3: Apply principle of statistical thermodynamics to understand the equilibrium phenomena.
CO4: Assess the importance of applications of statistical mechanics in related fields.

**Books and References**


1. Introduction to Statistical Thermodynamics by T.L. Hill, Addison-Wesley.
2. *S*tatistical Physics by L.D. Landau, E. M. Lifshitz, Butterworth-Heinemann.
3. Statistical Mechanics by A. McQuarrie, University Science Books.
4. Applied Statistical Mechanics by T.M. Reed, K.E. Gubbins, McGraw-Hill.
5. Thermodynamics and Statistical Mechanics by Attard, Academic Press, Elsevier.

Course Name : **Computational Fluid Dynamics**
Course Code : **CH-728**
Course Type : **Programme Elective-IV**

Contact Hours/Week: **4L** Course Credit: **04**

**Course Objectives**

- To understand the theory of governing equations representing fluid flow behavior.
- To impart knowledge in finite volume method to solve fluid mechanics problems.
- To enable the students to solve partial differential equations using iterative methods.

**Course Content**

Introduction and Principles of Conservation: CFD Applications, Comparison between numerical, analytical and experimental approaches, Modeling vs. Experimentation, Fundamental principles of conservation, Reynolds transport theorem, Conservation of mass; Conservation of linear momentum: Navier-Stokes equation, Conservation of Energy, General scalar transport equation. Classification of Partial Differential Equations and Physical Behavior: Mathematical classification of Partial Differential Equation, Illustrative examples of elliptic, parabolic and hyperbolic equations, Physical examples of elliptic, parabolic and hyperbolic partial differential equations; Finite Volume Method: Conceptual Basics and Illustrations through 1-D Steady State Diffusion Problems: Physical consistency, Overall balance, Finite volume Discretization of a 1-D steady state diffusion type problem, Composite material with position dependent thermal conductivity, Four basic rules for Finite volume discretization of 1-D steady state diffusion type problem, Source term linearization, Implementation of boundary conditions, Finite volume discretization of convection-diffusion problem: Central difference scheme, Upwind scheme, Exponential scheme and Hybrid scheme, Power law scheme, Generalized convection-diffusion formulation, Finite volume discretization of two-dimensional convection-diffusion problem, The concept of false diffusion, QUICK scheme; Discretization of Navier Stokes Equations: Discretization of the momentum equation: Stream Function-Vorticity approach and primitive variable approach, staggered grid and collocated grid, SIMPLE Algorithm, SIMPLER Algorithm; Turbulence Modeling: Important features of turbulent flow, Vorticity transport equation, Statistical representation of turbulent flows, Homogeneous turbulence and isotropic turbulence, General Properties of turbulent quantities, Reynolds average Navier stokes (RANS) equation, Closure problem in turbulence, Necessity of turbulence modeling, Different types of turbulence model, Eddy viscosity models, Mixing length model, Turbulent kinetic energy and dissipation, The $\kappa$-$\varepsilon$ model, Advantages and disadvantages of $\kappa$-$\varepsilon$ model, More two-equation models: RNG $\kappa$-$\varepsilon$ model and $\kappa$-$\omega$ model, Reynolds stress model (RSM), Large eddy Simulation (LES),Direct numerical simulation (DNS)

**Course Outcomes**

Upon successful completion of the course, the students will be able to

CO1: Get knowledge on theory of governing equations representing fluid flow behavior
CO2: Solve steady state diffusion and convection fluid flow problems using Finite volume method
CO3: Discretize Navier-Stokes equations by various algorithms.
CO4: Understand the concept of turbulence and its modeling

**Books and References**

1. An Introduction to Computational Fluid Dynamics: The Finite Volume Method by H. Versteeg, W. Malalasekera, Pearson.
2. Computational Fluid Mechanics and Heat Tranasfer by D.A. Anderson, J.C. Tannehill, R.H. Pletcher, CRC Press.
3. Computational Fluid Dynamics by K.A. Hoffmann, S.T. Chiang, Engineering Education.
4. Computational Fluid Flow and Heat Transfer by K. Muralidhar, T. Sundararajan, Narosa Publishing House, New Delhi.