# MASTER OF TECHNOLOGY IN CHEMICAL ENGINEERING



# CHEMICAL ENGINEERING DEPARTMENT Motilal Nehru National Institute of Technology, Allahabad Prayagraj-211004 (India)

August, 2020

# Course Structure and Evaluation Scheme: M. Tech. (Chemical Engineering)

# SEMESTER I:

S.	Subject Subject Name Weekly Load Credit Distr				ribution of marks out of 100					
No.	Code		L	т	Р	Cr	ТА	Mid Sem. Exam.	End Sem. Exam.	Total
1.	CH-21101	Advanced Chemical Engineering Thermodynamics	4	0	-	4	20	20	60	100
2.	CH-21102	Chemical Reactor Analysis and Design	4	0	-	4	20	20	60	100
3.	CH-21XXX	Elective-I	4	0	-	4	20	20	60	100
4.	CH-21XXX	Elective-II	4	0	-	4	20	20	60	100
5.	CH-21XXX	Elective-III	4	0	-	4	20	20	60	100
			20	0	-	20				

#### **SEMESTER II:**

S.	Subject	Subject Name	Weekly Load			Credit	Distribution of marks out of 100			
No.	Code		L	т	Ρ	Cr	ТА	Mid Sem. Exam.	End Sem. Exam.	Total
1.	CH-22103	Advanced Transport Phenomena	4	0	-	4	20	20	60	100
2.	CH-22201	Chemical Engineering Lab	-	-	6	4	50	-	50	100
3.	CH-22XXX	Elective-IV	4	0	-	4	20	20	60	100
4.	CH-22XXX	Elective-V	4	0	-	4	20	20	60	100
5.	CH-22XXX	Elective-VI	4	0	-	4	20	20	60	100
			16	0	6	20				

#### SEMESTER III:

S. No.	Subject Code	Subject Name	Credit	Evaluation out of 100 marks
1.	CH-23651	Special Study/Term Project/State of the art/ Colloquium/Industrial/Research Training	4	Marks
2.	CH-23602	Thesis/Project	16	Marks

#### **SEMESTER IV:**

S. No	Subje . Code		Name Credit	Evaluation out of 100 marks
1	CH-246	03 Thesis/Project	20	Marks

Total Credits = 20 (I) + 20 (II) + 20 (III) + 20 (IV) = 80

List of Electives – (Semester I)				
S. No.	Code	Name of Elective		
1.	CH-21301	Mathematical methods in Chemical Engineering		
2.	CH-21302	Advanced Process Dynamics and Control		
3.	CH-21303	Energy and Environment		
4.	CH-21304	Multicomponent Mass Transfer		
5.	CH-21305	Polymer Science and Technology		
6.	CH-21306	Petroleum Refinery Engineering		
7.	CH-21307	Modeling and Simulation		
8.	CH-21308	Process Optimization		
9.	CH-21309	Advanced Heat Transfer		
10.	AM-21102	Applied Mathematics and Computations		
11.	AM-21106	Computational Fluid Dynamics		
12.	AM-21346	Multiphase Flow		
		List of Electives – (Semester II)		
1.	CH-22401	Novel Separation Processes		
2.	CH-22402	Multi-Phase Flow and Heat Transfer		
3.	CH-22403	Process Intensification		
4.	CH-22404	Petrochemical Technology		
5.	CH-22405	Nuclear Engineering		
6.	CH-22406	Process Safety and Hazards Management		
7.	CH-22407	Fundamentals of Biochemical Engineering		
8.	CH-22408	Experimental Design and Data Analysis		
9.	CH-22409	Colloids and Interfacial Engineering		
10.	AM-22102	Characterization of Materials		
11.	CE-22121	Principles of Biological Waste Water Treatment		
12.	CE-22358	Environmental Impact Assessment		

# ADVANCED CHEMICAL ENGINEERING THERMODYNAMICS [CH-21101] [L:T:P:Cr = 4:0:0: 4]

**Objective:** This course aims to provide insight on phase equilibrium thermodynamics for multi-component systems. A part of the course is devoted to statistical mechanics and its relation to thermodynamics. **Prerequisites:** Basic knowledge of thermodynamics and chemical engineering thermodynamics.

#### **COURSE OUTLINE**

#### Unit I

Review of fundamental principles: Review of thermodynamic laws, thermodynamic potentials, thermodynamic stability, and thermodynamic properties of pure substances.

#### Unit II

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.

#### Unit III

Phase equilibria: Fundamental VLE equation, VLE at low, moderate and high pressures, azeotropic data, multicomponent VLE, thermodynamic consistency test of VLE data, liquid-liquid equilibria, chemical reaction equilibria.

#### Unit IV

Intermolecular forces: Interactions between molecules, electrostatics and dipoles, potential-energy functions, molecular dynamics simulations.

#### Unit V

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.

#### **Text/Reference Books**

- 1. Prausnitz, J.M.; Lichtenthaler, R.N.; Gomes de Azevedo, E. "Molecular Thermodynamics of Fluid Phase Equilibria", Prentice Hall, 3<sup>rd</sup> Edition, 1998.
- 2. Sandler, S.I. "Chemical, Biochemical and Engineering Thermodynamics", Wiley, 4<sup>th</sup> Edition, 2006.
- 3. Rao, Y.V.C. "Chemical Engineering Thermodynamics", Universities Press, 1997.
- Smith, J.M.; Van Ness, H.C.; Abbott, M.M. "Introduction to Chemical Engineering Thermodynamics", MGHFSE, 7<sup>th</sup> Edition, 2005.
- 5. Koretsky, M.D. "Engineering and Chemical Thermodynamics", Wiley, 2004

# SEMESTER I

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# CHEMICAL REACTOR ANALYSIS AND DESIGN [CH-21102] [L: T: P: Cr = 4:0:0:4]

**Objective:** The objective is to enable understanding of design of industrially important reactors both for homogeneous and heterogeneous chemical reactions on a commercial scale.

**Prerequisite:** Basics of chemical reaction engineering along with the fundamental knowledge of mass and heat transfer.

#### **COURSE OUTLINE**

# Unit I:

Introduction to Chemical Reaction Engineering: chemical reactions, reaction order, molecularity, conversion, rate law and stoichiometry, elementary and non- elementary reactions, reaction rate constant, chemical equilibrium. Design of Isothermal Reactors: batch reactor, continuous stirred tank reactor (CSTR), plug-flow tubular reactor (PFTR), semi-batch reactor and recycle reactors.

#### Unit II:

Design of Non-isothermal Reactor: energy balance, reactors heat generation and removal, non isothermal continuous flow reactor, energy balance in a CSTR and PFTR, adiabatic reactors, trajectories and phase-plane plots, trajectories of wall-cooled reactors.

# Unit III:

Catalyst & Catalysis: catalytic reactions, reaction rates, rate equation for surface kinetics, porous catalysts, pore diffusion, and temperature dependence of catalytic reaction rates. Design of packed bed reactor for catalytic reactions

# Unit IV:

Multiphase Reactors: introduction, types, and mass balance equations for multiphase reactors, interfacial surface area, mass transfer between phases, equilibrium between phases, membrane reactors, falling film reactor, bubble column reactors, trickle bed reactor, slurry reactor.

#### Unit V:

Models for Non-ideal Reactors: basics of non-ideal flow, residence time distribution (RTD) in ideal reactors; residence time distribution (RTD) in non-ideal reactors, Tanks-in-Series (T-I-S) model, Dispersion model, reaction and dispersion, Tanks-in-Series model versus Dispersion model.

#### **Text/Reference Books**

- Froment, G. F., Bischoff, K. B., and Wilde, J. D., "Chemical Reactor Analysis and Design", 3<sup>rd</sup> Edition, John Wiley & Sons, 2010.
- 2. Levenspiel, O., "Chemical Reaction Engineering", 3<sup>rd</sup> Edition, John Wiley & Sons, 2004.
- 3. Fogler, H. S., "Elements of Chemical Reaction Engineering" 3rd Edition, Prentice-Hall of India, 2005.
- 4. Schmidt, L. D., "The Engineering of Chemical Reactions", 2<sup>nd</sup> Edition, Oxford University Press, 2005.

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# SEMESTER II

# ADVANCED TRANSPORT PHENOMENA [CH-22103] [L:T:P:Cr = 4:0:0:4]

**Objective:** To develop an understanding of momentum, heat and mass transport in Chemical Engineering as well as in process industries.

**Prerequisites:** Basic knowledge of undergraduate chemical engineering courses particularly heat transfer, mass transfer and fluid mechanics.

#### **COURSE OUTLINE**

#### Unit I

Fundamentals of transport processes, basics of vector and tensor algebra, phenomenological equations and transport properties, analogies amongst momentum, heat, and mass transport; Non-Newtonian fluids and rheological behaviour.

#### Unit II

Basic transport equations for isothermal, non-isothermal and multicomponent systems; velocity, temperature and concentration distributions with more than one independent variables; velocity, temperature and concentration distributions in laminar and turbulent flow.

#### Unit III

Macroscopic balances for isothermal, non-isothermal and multicomponent system and their applications in momentum, heat and mass transport problems; simultaneous momentum, heat and mass transfer with chemical reaction.

#### Unit IV

Analytical methods for solution of transport equations

#### Unit V

Computational methods involve in multiphase flow, chemically reacting flows, turbulent mixing etc.

#### **Texts/References:**

- 1. Bird, R.B., Stewart, W.E. and Lightfoot, E.N., "Transport Phenomena", 2<sup>nd</sup> Edition, John Wiley & Sons, 2002.
- 2. Deen, W.M., "Analysis of Transport Phenomena", Oxford University Press, 1st Edition, 2008.
- 3. Slattery, J., "Advanced transport phenomena", Cambridge University Press, 1999.
- 4. Leal, L. "Advanced Transport Phenomena: Fluid Mechanics and Convective Transport Processes", Cambridge University Press, 2007.
- 5. Geankoplis C.J. "Transport Processes and Separation Process Principles" Prentice Hall, 2003

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#### CHEMICAL ENGINEERING LAB [CH-22201]

#### 1. ADVANCED MODELLING AND SIMULATION LABORATORY

- I. Steady state and Dynamic simulation using ASPEN PLUS software package.
- II. Simulation of flowing systems channel using ANSYS software package.
- III. VLE/LLE using COSMOtherm software.

#### 2. ANALYTICAL LAB

- I. To perform the experimental analysis on Gas Chromatography (GC).
- II. To perform measurements using UV Vis spectrophotometer.
- III. To perform the experimental analysis on High Performance Liquid Chromatography (HPLC).
- IV. To analyze the samples using XRD, SEM and EDX.

#### 3. PROCESS ENGINEERING LABORATORY

#### a. Advanced Chemical Reaction Engineering Laboratory

- 1. To perform the experiment on CSTRs connected in series.
- 2. To perform the experiment on PFRs connected in series.
- 3. To study RTD, flooding characteristics and pressure drop in a packed bed reactor.

#### b. Advanced Mass Transfer/ Advanced Chemical Engineering Thermodynamics Laboratories

- 1. Vapour-liquid equilibrium (VLE) study
- 2. Liquid-liquid equilibrium (LLE) study.
- 3. Determination overall mass transfer co-efficient and individual height of transfer unit based on continuous & dispersed phase.
- 4. To estimate number of theoretical stages in distillation column.

# PROFESSIONAL ELECTIVES (SEMESTER-I)

# **MATHEMATICAL METHODS IN CHEMICAL ENGINEERING [CH-21301]** [L:T:P:Cr = 4:0:0:4]

**Objective:** The present course aims to help the student to learn, different mathematical technique to solve and analyze different classes of Chemical Engineering problem.

Prerequisites: Knowledge of basic chemical engineering courses and general mathematics for applying in chemical engineering problems.

#### **COURSE OUTLINE**

#### Unit I

Introduction of vector space, metrics, norms, inner products, normed linear space, dimension of vector spaces, applications, linear combination of vectors, dependent/independent vectors, Orthogonal and orthonormal vectors, Gram-Schmidt Orthonormalization.

#### Unit II

Basics of matrix, determinants and properties, Eigenvalue and Eigenvector problems, various theorems, solution of a set of algebraic equations, solution of a set of algebraic equations, solution of a set of ordinary differential equations, solution of a set of non-homogeneous ordinary differential equations (IVPs), Rayleigh's quotient, non self adjoint systems.

#### Unit III

Partial differential equations, Classification of equations, boundary conditions, principal of linear superposition, developing PDE in chemical engineering systems, infinite dimensional spaces, Solution of linear homogeneous PDE's by separation of variables, Cartesian coordinate system, cylindrical & spherical coordinate systems, solution of PDE's by finite Fourier transformation.

#### Unit IV

Various applications of ODE & PDE in chemical engineering systems, maximum principles, energy methods, Fredhalm alternative, monotone iteration method, numerical analysis, method of continuation.

#### Unit V

Application of Eigenvalue problems, Stability analysis, bifurcation theory, Landau-Hopf scenario, period doubling cascades, Ruelle- Takens scenario, characteristic of trajectories.

#### **Text/Reference Books**

- 1. Pushpavanam, S. "Mathematical Methods in Chemical Engineering" PHI, New Delhi, 1998.
- 2. Rice, R.G. & Do, D.D. "Applied Mathematics and Modelling for Chemical Engineers" John Wiley and Sons,2<sup>nd</sup> Edition, 2012.
- 3. Verma, A. & Morbidelli, M. "Mathematical modelling in Chemical Engineering" Oxford University Press, New York, 1997.
- 4. Loney, N.W. "Applied Mathematical Methods for Chemical Engineers" CRC Press, 2<sup>nd</sup> Edition, 2006.
- 5. Gupta, S.K. "Numerical Methods for Engineers" New Age International, New Delhi, 1995.

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# ADVANCED PROCESS DYNAMICS AND CONTROL [CH-21302] [L:T:P:Cr = 4:0:0:4]

**Objective:** The objective of this course is to provide a fundamental understanding to develop a technology for chemical processes.

Prerequisites: Knowledge of process dynamics and control

#### **COURSE OUTLINE**

# Unit I

Classical controllers, controller tuning and stability analysis, feedback control of systems with dead-time, interaction of control loops,

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#### Unit II

Process identification and adaptive control, Z-transforms, phase-plane analysis, bifurcation behaviour, linearization via variable transformation

# Unit III

Dynamic matrix control, quadratic dynamic matrix control, model algorithmic control, nonlinear model predictive control.

# Unit IV

Generic model control, globally linearizing control, inferential control, internal model control, model-reference adaptive control.

# Unit V

Open-loop estimator, Kalman filtering, Luenberger estimator, inferential estimator, principal component regression, controller design, fuzzy estimator, multivariable control.

#### **Text/ Reference Books**

- 1. Bequette, B. W. "Process Control: Modeling, Design, and Simulation," Prentice-Hall of India Private Limited, New Delhi, 1<sup>st</sup> ed., 2003.
- Chidambaram, M. "Computer Control of Processes," Narosa Publishing House, New Delhi, 1<sup>st</sup> ed., 2002.
- Seborg, D.E.; Edgar, T.F.; Mellichamp, D.A. "Process Dynamics and Control," John Wiley & Sons, Inc., New Jersey, 2<sup>nd</sup> ed., 2004.
- 4. Ogunnaike, B.A.; Ray, W.H. "Process Dynamics, Modeling, and Control," Oxford University Press, New York, 1<sup>st</sup> ed., 1994.
- 5. Stephanopoulos, G. "Chemical Process Control: An Introduction to Theory and Practice," PHI Private Limited, New Delhi, 1<sup>st</sup> ed., 1984.

#### **ENERGY AND ENVIRONMENT [CH-21303]**

### [L:T:P:Cr = 4:0:0:4]

**Objective:** The objective of this study is to expose the students to latest techniques used to safeguard our environment. This course will cover state of the art methods currently used in the field of energy and environment.

Prerequisites: Knowledge of basic chemical engineering.

#### **COURSE OUTLINE**

#### Unit I

Climate change, global warming, cause and consequence of climate change.  $CO_2$  emissions from various sources, options available to counter climate change.

#### Unit II

 $CO_2$  capture,  $CO_2$  transportation,  $CO_2$  storage, different types of storage options, ocean storage, storage in geological formation such as deep saline formation and depleted oil reserves,  $CO_2$  leakage, economic of CCS with examples around the world, biological sequestration, mineral sequestration,  $CO_2$  utilization, India CCS scenario.

#### Unit III

Fuel cell principles, fuel cell technology research, thermodynamics related to fuel cell, fuel cell systems, system design, power generation based on fuel cells, case study related to fuel cells.

#### Unit IV

Overview of hydrogen based economy, production of hydrogen, storage and handling of hydrogen, environmental concerns related to hydrogen, hydrogen energy.

#### Unit V

Wind energy, types of wind turbines, solar energy, solar photovoltaics, research and development status of solar energy, case studies.

#### **Text/Reference Books:**

- 1. Masters, G.M.; and Ela W.P. "Introduction to Environmental engineering and Science" EEE publication, 2005.
- 2. Ristinen, R.A.; and Kraushaar, J.J. "Energy and the Environment" John Wiley & Sons, Inc., USA, 2005.
- 3. Boyle, G.; Everett, B.; and Ramage, J. (Editors) "Energy Systems and Sustainability: Power for a Sustainable Future" Oxford University Press, UK, 2003.
- 4. Jennifer W. "Carbon Capture", Springer, 2012.
- 5. Basu S. "Recent Trends in Fuel Cell Science and Technology", Springer, 2007.

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# MULTI COMPONENT MASS TRANSFER [CH-21304] [L:T:P:Cr = 4:0:0:4]

**Objective:** To emphasize on the concepts used in distillation absorption and extraction operations for multicomponent mass transfer.

Prerequisites: Basic course of mass transfer

#### **COURSE OUTLINE**

#### Unit I

Introduction: Overview of binary systems: Gibbs phase rule, flash, bubble point and dew point calculations, diffusive, equilibrium and rate based methods.

#### Unit II

Multicomponent cascade systems: Cascade configurations, liquid-liquid extraction cascades, vapour liquid cascades, membrane cascades, specifications for counter current cascades.

#### Unit III

Approximate methods for multicomponent-multistage separation: Fenske-Underwood-Gilliland method, Fenske equation for minimum equilibrium stages, Underwood equations for minimum reflux, Gilliland correlation for actual reflux ratio and theoretical stages, Kramser Group method for strippers and liquid-liquid extraction.

#### Unit IV

Equilibrium based methods for multi-component systems: Theoretical model for equilibrium stage, general strategy of mathematical solution, equation –tearing procedure: Bubble point method for distillation, sum rates method for absorption and stripping, Newton Raphson method, MESH equations.

#### Unit V

Design of multicomponent systems: Design of multicomponent distillation column using Lewis-Matheson method, azeotropic and extractive distillation, reactive multistage separations, diffusion in non-ideal system and development of generalized Maxwell-Stefan formulation, Study of generalized Fick's law.

#### **Text/Reference Books:**

- 1. Seader J. D.; Henly E. J., Separation Processes and Principles, John Wiley, 2010, 3<sup>nd</sup> edition.
- 2. Taylor R.; Krishna R., Multicomponent Mass Transfer, John Wiley, 1993.
- 3. Bendaitez J. Principles and Modern Applications of Mass Transfer Operations, Wiley, 2<sup>nd</sup> edition, 2011.
- 4. Holland, C. D. Fundamentals of Multicomponent Distillation, McGraw Hill, 1981.
- 5. Wankat P. C., Separation Process Engineering, Prentice Hall, 2011, 3<sup>nd</sup> edition.

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# POLYMER SCIENCE AND TECHNOLOGY [CH-21305] [L:T:P:Cr = 4:0:0:4]

**Objective:** This course is designed to learn the fundamentals of polymer technology from the basics to more advanced topics such as structure-property relationships, solution thermodynamics, polymer mechanical properties, polymer rheology, etc.

#### **COURSE OUTLINE**

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#### Unit –I

Classification of polymers: Natural and synthetic polymers, thermosets and thermoplasts, copolymers, terpolymers, degradable and non-degradable polymers

#### Unit-II

Micro-structure of polymer chains: Configuration and conformation, simple and hindered rotation, molecular weight distribution of polymers, crystallinity and melting, glass transition temperature, physical states of polymers and mode of motion of polymer chains, measurement of viscosity, cohesive energy density, compatibility and solubility parameters, polymer additives, blends and composites.

#### **Unit-III**

Addition polymerization, condensation polymerization, ring opening polymerization, copolymerization, polymerization by coordination catalyst.

#### Unit-IV

Flow properties of polymers: Bulk deformation, elongation and shear flow, non-Newtonian flow. Polymer fabrication techniques: Formation of flat sheets and films, laminations, foam formation, extrusion, injection moulding, blow moulding, compression and transfer molding, spinning of fibres

# Unit-V

[8] Manufacturing processes of important polymers: plastics, rubbers, elastomers, fibres, polymeric oils, conducting polymers, smart polymers, ecology and environmental aspects of polymer industries

#### **Text/Reference Books:**

- 1. Joel R. Fried, "Polymer Science and Technology", Prentice Hall of India, Pvt. Ltd., New Delhi, 1995
- 2. Ferdinand Rodriguez, "Principles of Polymer Systems", Taylor & Francis Washington D.C., 4th ed., 1996.
- 3. Tadmore, and Gogvs, C.G., "Principles of Polymer Processing" John Wily & Sons.
- 4. Fred W. Billmeyer, Jr, "Textbook of Polymer Science", John Wiley & Sons, New York, 3rd ed., 1994.
- 5. Alfred Rudin, "Polymer Science and Engineering", Academic Press, USA, 2<sup>nd</sup> ed., 1999.

# **PETROLEUM REFINERY ENGINEERING [CH-21306]** [L:T:P:Cr = 4:0:0:4]

**Objective:** To provide fundamental understanding of petroleum refining processes and update about the latest developments and emerging operations in the downstream hydrocarbon sector.

Prerequisite: General idea about crude oil and petroleum refining products.

#### **COURSE OUTLINE**

#### Unit I

World and Indian reserves of crude oil, Indian exploration and production (E&P) scenario, global and indian petroleum refining scenario, composition of crude oil, classification of crude oil, types of refineries, fuel refinery, lube refinery, various petroleum products, Indian specifications, testing methods and their significance. [5L]

#### Unit II

Dehydration and desalting of crude oil, descriptive account of atmospheric distillation, vacuum distillation, various straight run products, properties and applications, treatment of important product.

#### Unit III

Thermal conversion processes: reaction mechanism of thermal processes, free radical mechanism, thermal cracking, coil visbreaking, soaker visbreaking, aquaconversion, delayed coking, fluid coking, flexi coking (reactions, operating variables, various designs proposed by technology supplier for each of these processes). Unit IV [9L]

Catalytic conversion processes: reaction mechanism of catalytic conversion processes, carbonium ion mechanism, catalytic cracking, fixed bed and moving bed catalytic cracking and fluidized catalytic cracking, deep catalytic cracking, hydrocracking, catalytic reforming, isomerisation, alkylation (reactions, catalyst used, operating variables, various designs proposed by technology supplier for each of these processes)

#### Unit V

Emerging operations in petroleum refineries, bottom-of-the-barrel upgradation, petroleum coke gasification, Fischer-Tropsch synthesis for the production of synthetic hydrocarbons (transportation fuels) from synthesis gas, integrated gasification combined cycle for power generation from synthesis gas.

#### **Text/Reference Books:**

- 1. Hobson, G.D.; Pohl W. "Modern Petroleum Technology", Wilev & Sons Publication, 4th Edition, 1973.
- 2. Speight, J.G. "The Chemistry and Technology of Petroleum", Marcel Dekker Publication, 4th Edition, 2006.
- 3. Gary J.H.; Handwerk, G.E.; Kaiser, M.J. "Petroleum Refining: Technology and Economics", Marcel Dekker Publication, 5<sup>th</sup> Edition, 2007.
- 4. Watkins, R.N. "Petroleum Refinery Distillation," *Gulf Pub. Co. Publication*, 1<sup>st</sup> Edition, 1973.
- 5. Bland W.E.; Davidson P.L. "Petroleum Processing Handbook", McGraw Hill Publication, 1967.
- 6. Nelson, W.L., "Petroleum Refinery Engineering", *McGraw Hill* Publication, 1<sup>st</sup> Edition, 1958.

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# **MODELING AND SIMULATION (CH-21307)**

L: T: P: Cr = 3:1:0:4

#### **COURSE OUTLINE**

Introduction to modeling and simulation, classification, Uses of mathematical models, Principles of model formulation, Fundamental laws- continuity equation, energy equation, equations of motion, Transport equations, equations of state, equilibrium and kinetics, Introduction to process simulators and mathematical tools.

#### UNIT 2

Numerical solution of model equations with linear and non linear algebraic equations in one and more than one variables, ordinary differential equations in one and more than one variables

#### UNIT 3

Numerical solutions of model equations with partial differential equations using finite difference method, Model parameters estimation: Introduction, method of least squares, curve fitting, etc.

#### UNIT 4

Lumped Parameter Models: Formulation and solution techniques for vapor-liquid equilibrium models, batch and continuous distillation column, mixing tank, stirred tank with heating, CSTR with multiple reactions. N- CSTRs in series, Non-isothermal CSTR.

#### UNIT 5

Steady State Distributed Parameter Models: Formulation and solution of split boundary value problems - shooting technique, quasi-linearization techniques, counter current heat exchanger, tubular reactors.

#### UNIT 6

Unsteady State Distributed Parameter Models: convective problems, diffusive problems, combined convective and diffusive problems.

#### **TEXT & REFERENCE BOOKS:**

- 1. K. M. Hangos and I. T. Cameron, "Process Modeling and Model Analysis", Academic Press, 2001.
- W.L. Luyben, "Process Modelling, Simulation and Control for Chemical Engineers", 2<sup>nd</sup> Edn., McGraw Hill Book Co., New York, 1990.
- 3. W. F. Ramirez, "Computational Methods for Process Simulation", Butterworths, 1995.
- 4. Singiresu S. Rao, "Applied Numerical Methods for Engineers and Scientists" Prentice Hall, Upper Saddle River, NJ, 2001

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# PROCESS OPTIMIZATION [CH-21308] [L:T:P:Cr = 4:0:0:4]

**Objective:** The present course aims the study of optimization techniques for designing any chemical process, and the principles for developing an executive system.

Prerequisites: Numerical methods and other UG level chemical engineering courses

#### **COURSE OUTLINE**

#### Unit I

Introduction to optimization; formulation of objective function; basic concepts-functions, regions, necessary and sufficient conditions for an extreme of an unconstrained function; one dimensional search: scanning and bracketing; Newton, quasi-Newton and secant methods; region elimination method, polynomial approximation methods.

#### Unit II

Unconstrained multivariable optimization: Direct methods-random search, grid search, univariate search, simplex method, conjugate search direction and Powell's method; Indirect method-gradient and conjugate gradient methods. Newton's method, movement in search direction, secant method.

#### Unit III

Linear programming: Basic concept in linear programming; Graphical solution; simplex method; Standard LP from; Obtaining first feasible solution; Sensitivity analysis. Non linear programming: Lagrange multiplier method; Quadratic programming; penalty function and augmented Lagrangian methods; Successive quadratic programming; Optimization of dynamic process.

#### Unit IV

Optimization of staged and discrete processes: Dynamic programming; integer and mixed integer programming; Non traditional optimization techniques: Simulated anneling; Genetic algorithms; Differential evolution.

#### Unit V

Application of optimization in the design of separation process, chemical reactor and large scale process plant.

#### **Text/Reference Books:**

- 1. Onwubolu, G. C.; Babu, B. V., "New Optimization Techniques in Engineering; Springer-Verlag, Germany, (2004).
- 2. Babu, B. V. "Process Plant Simulation", Oxford University Press, India (2004).
- 3. Jana A. K., "Chemical Process Modeling and Computer Simulation" PHI, New Delhi (2011)

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# **ADVANCED HEAT TRANSFER [CH-21309]** [L: T: P: Cr = 4:0:0:4]

**Objective:** The present course aims to help the student to understand various heat transfer mechanism in unsteady state and advances in convection, turbulent flows and radiation.

**Prerequisites:** Knowledge of basics of conduction, convection, radiation and heat transfer equipments design.

#### **COURSE OUTLINE**

Heat condition: Introduction, extended surfaces, lumped system analysis, transient heat conduction in large plane walls, long cylinders and spheres, transient heat conduction in semi-infinite solids, numerical solution of multi-dimensional conduction problems, transient heat conduction charts.

#### Unit II

Unit I

Convection: convective heat transfer-theories and practices, laminar boundary layer on a flat plate, energy equation for thermal boundary layer over a fiat plate, momentum and heat exchange in turbulent fluid flow, flow across spheres, cylinders and tube banks.

#### Unit III

Heat transfer with phase change: Boiling- regimes of pool boiling and heat transfer during boiling, Condensation- drop wise and film wise condensation, effect of turbulence and high velocity on film wise condensation.

#### Unit IV

Heat exchanger design: Basic design procedure and theory - overall heat transfer coefficients, fouling factors; type of heat exchangers- shell and tube, plate, direct contact, finned tubes, air cooled and Compact heat exchangers, Efficiency of heat exchangers and number of transfer units, (N.T.U.)

#### Unit V

Heat transfer in packed bed, fluidized bed and nuclear reactors - basic fundamental and factors affecting the rate of heat transfer, heat transfer in liquid metals,

#### **Text/Reference Books**

- 1. Sinnott, R. and Towler, G., "Chemical Engineering Design", Vol. 6, Coulson & Richardson's Chemical Engineering Series, 5<sup>th</sup> Eddition, Elsevier, 2009
- 2. Holman, J. P., Heat Transfer, Tata McGraw Publication, 9th Edition, 2002.
- 3. Tong, L. S., and Tang, Y. S., "Boiling Heat Transfer and Two-Phase Flow", 2<sup>nd</sup> Edition, Taylor& Francis 1997.
- 4. S. G. Kandlikar, "Handbook of Phase Change: Boiling and Condensation" Taylor & Francis, 1999.

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#### APPLIED MATHEMATICS AND COMPUTATIONS [AM-21101] [L:T:P:Cr = 4:0:0:4]

#### **COURSE OUTLINE**

#### Introduction: [5 L] Motivation, Mathematical modeling, Errors in numerical methods, Convergence, Conditioning and stability. **Nonlinear Equations:** [5 L] Motivation, Open and braketing method, Bisection, Fixed point, Newton's method, Secant and False position method, Rate of convergence, Merits and demerits of methods. **Simultaneous Linear Equations:** [5 L] Motivation, Gauss elimination, Pivoting, Factoring, Solution accuracy, Iterative methods, Jacobi method, Gauss-Siedel method, Relaxation method. **Interpolation and Curve Fitting:** [6 L] Motivation, Polynomial forms, Linear interpolation, Lagrangean interpolation, Newton interpolation, Spline interpolation, Chebyshev interpolation, Regression analysis, fitting linear equations, Least-square method, Fitting transcendental equations, Polynomial functions, Multiple linear regression. **Simultaneous Non-Linear Equations:** [4 L] Motivation, Successive substitution method, Newton's method. **Numerical Integration:** [5L] Motivation, Newton-Kotes method, Trapezoidal rule, Simpson's rule, Rhomberg integration, Gauss Quadrature. **Initial Value Problem:** [5 L] Motivation, Euler's method, Modified Euler method, Runge-Kutta methods, Adaptive integrations and multistep methods **Boundary-value and Eigen-value Problem:** [5 L]

Motivation, Shooting method, Finite difference method, Finite volume method, Polynomial method, Power method, Elliptic, Parabolic and Hyperbolic Partial Differential Equations.

#### Text & References

1. "Applied Numerical Analysis", C.F. Gerald and P.O. Wheatley, 5th edition, Addison-Wesley, 1998.

2. "Numerical Mathematics & Computing", W. Cheney and D. Kincaid, 5th edition, Brooks/Cole, 2004.

3. "Applied Partial Differential Equations", Paul DuChateau and David Zachmann.

4. "Partial Differential Equations for Scientists and Engineers", Stanley J. Farlow.

5. "Numerical Methods for Partial Differential Equations", William F. Ames.

6. "Numerical Methods for Elliptic and Parabolic Partial Differential Equations", John R Levison, Peter Knabner, Lutz Angermann .

#### **COMPUTATIONAL FLUID DYNAMICS [AM-21106]** [L:T:P:Cr = 4:0:0:4]

#### **COURSE OUTLINE**

#### **Basic ideas of CFD:**

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

#### **FVM for Diffusion Problems:**

FVM for 1D steady state diffusion, 2D steady state diffusion, 3d steady state diffusion. Solution of discretised equations - TDMA scheme for 2D and 3D flows.

#### **FVM for Convection-Diffusion Problems:**

FVM for 1D steady state convection-diffusion, Central differencing scheme, Conservativeness, Boundedness, Transportiveness, Upward differencing scheme, Hybrid differencing scheme for 2D and 3D convectiondiffusion, Power-law scheme, QUICK scheme.

Solution Algorithm for Pressure-velocity Coupling in Steady Flows: [4L]

Concept of staggered grid, SIMPLE, SIMPLER, SIMPLEC, PISO algorithm.

#### **Grid Generation:**

General transformation of the equations. Metices and Jacobians. Types of grids- structured and unstructured grids, grid generation methods- algebraic, differential and hybrid methods. Coordinate stretching, boundaryfitted coordinate systems. Elliptic and hyperbolic grid generation methods, orthogonal grid generation for Navier-Stokes equations, Multi-block grid generation.

#### Introduction to turbulence modeling:

Reynolds averaged N-S equations, various turbulence models- mixing length, k-epsilon, Reynolds stress. Boundary conditions, paraboloid N-S equations, direct numerical simulations (DNS) and large-eddy simulation, sub-grid models, pseudo-spectral method, examples.

#### **Text & References:**

- 1. "An Introduction to Computational Fluid Dynamics: the Finite Volume Method", H.K. Versteeg and W. Malalasekera, Longman Scientific & Technical, 1995/Addison-Wesley, 1996.
- 2. "Computational Fluid Flow and Heat Transfer" (2ndedition), K. Muralidhar and T. Sundararajan, Narosa Publishing, 2004.
- 3. "Numerical Heat Transfer and Fluid Flow", S.V. Patankar, McGraw-Hill, New York, 1980.
- 4. "Computational Methods for Fluid Dynamics" (3rdedition), J.H. Ferziger and M. Peric, Springer, 2001.
- 5. "Fundamentals of Computational Fluid Dynamics", T. K. Sengupta, Universities Press, Hyderabad, 2004.

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# MULTIPHASE FLOW [AM-21346] [L:T:P:Cr = 4:0:0:4]

#### **COURSE OUTLINE**

UNIT – 1 [5 L]
Introduction to Multiphase Flow: History of multiphase flow investigation, Multiphase Flow in Engineering,
Parameters, characterizing multiphase flow.
UNIT – 2 [6 L]
Classification of Multiphase Flow: Flow Patterns (Solid-Liquid, Solid-Gas, Gas- Liquid), Dispersed flow,
intermittent flow, Separated flow.
UNIT – 3 [4L]
Basic Equation: Mass, momentum and energy conservations, Constitutive law.
UNIT – 4 [7 L]
Cavitation Phenomena: Homogeneous flow, Bubbly flow, Separated flow, Intermittent flow, Inception and
Cavitation Nuclei, Bubble Dynamics, Developing Process of Cavitation, Cavitation Characteristics.
UNIT – 5 [12 L]
Numerical Methods for Complex Multiphase Flow: Mathematical Modeling- Homogeneous flow model, Drift-
flux model, Two-fluid model, Void fraction and pressure drop estimation, Homogeneous flow model, Separated
Flow model. Mathematical Modeling and Numerical Analysis of Gas-Liquid Two-Phase Flow. Numerical
Simulation of Cavitating Flow. Wave propagation, Flow instability, Flow pattern transition, Ledinegg type flow
instability.
<u>UNIT-6</u> [6L]

Slurry Pumps: Design & uses, Recent advancement in multiphase flow.

#### Text and references:

1. "Multiphase Fluid Flow Theory & Practice", F.G. Hammitt, McGraw -Hill Inc., NY, 1980.

2."The Flow of Complex Mixtures in Pipes", G.W. Govier & K. Aziz, Van Nostrand Reinhold Co., NY, 1972.

# **PROFESSIONAL ELECTIVES (SEMESTER-II)**

#### **NOVEL SEPARATION PROCESSES [CH-22401]**

### [L:T:P:Cr = 4:0:0:4]

**Objective:** to study the advancements in existing adsorptive separation and some new separation technologies. The students will take up projects related to the application of these technologies in chemical and allied industries.

Prerequisites: Basic course of mass transfer

#### **COURSE OUTLINE**

### Unit I

Introduction: Review of conventional processes, various separation processes, classification of separation processes such as diffusion and rate based separations.

#### Unit II

Adsorptive separation: Fixed-bed and moving bed adsorption, thermal swing and pressure swing adsorption methods for regeneration, parametric pumping, mathematical modelling of adsorption process, chromatographic techniques.

#### Unit III

Membrane based separations: Concepts of membrane separation, membrane materials, synthesis and characterization of membranes, modules, transport in membranes, methods for liquid and gaseous separations, pervaporation, liquid membranes and membrane reactors.

#### Unit IV

Bio-separation: Concept, Introduction to bio-kinetics, types of bio-reactors, different techniques for bioseparation, modeling approach, design considerations and applications

#### Unit V

Other Techniques: Supercritical fluid extraction - Concept, modelling, design aspects and applications, separations using surfactants.

#### **Text/Reference Books:**

- 1. Mulder J., Basic Principles of membrane Technology, Springer, 1996.
- 2. Wankar P. C., Large Scale Adsorption and Chromatography, CRC, 1986.
- 3. Ruthven D. M., Principles of Adsorption and Adsorption Processes, John Wiley, 1984.
- 4. Sourirajan S., Matsuura T., Reverse Osmosis and Ultra-Filtration Process Principles, NRC Publication, Ottawa, 1985.
- 5. McHugh M. A., Krukonis V.J, Supercritical Fluid Extraction, Butterworth, 1985.
- 6. Seader J. D., Henly E. J., Separation Processes and Principles, John Wiley, 2010
- 7. Osadar, Nakagawa V., Membrane Science and Technology, Marcel Dekkar, 1992

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# MULTI PHASE FLOW AND HEAT TRANSFER [CH-22402] [L: T: P :Cr = 4:0:0:4]

**Objective:** The course has been designed to give a thorough understanding of mechanism involved in multiphase flow and heat transfer with special emphasis on heat transfer with phase changes - boiling & condensation.

Prerequisites: Basic knowledge of fluid mechanics and heat transfer at under graduate level.

#### Unit-I

Introduction to Multi Phase Flow: type and applications, flow patterns in adiabatic flow, flow pattern transitions in adiabatic flow, flow patterns in diabatic flow, void fraction and slip ratio, methods of identifications and measurement techniques for flow regimes. Introduction to multi-phase flow problems in process industry, multi-phase flow with heat transfer.

**COURSE OUTLINE** 

#### Unit-II

Modelling of Multi-Phase Flow: homogeneous model/drift flux model, separate-phase model (two-fluid model), models for flow pattern transition, models for bubbly flow, models for slug flow, models for annular flow, models for stratified flow (horizontal pipes), transient models. Pressure drop models in multi-phase flow systems.

# Unit-III

Heat Transfer with Phase Change – Boiling: modes of pool boiling, boiling curve, heat transfer mechanism in pool boiling: bubble nucleation, growth and departure from a heated surface, bubble emission frequency, waiting period, correlation of nucleate boiling data, pool boiling crisis, film boiling in a pool; forced convection boiling, burnout.

# Unit-IV

Heat Transfer with Phase Change – Condensation: type of condensation, film condensation, drop-wise condensation, condensation on a vertical plate, condensation on tubes and spheres.

# Unit-V

Heat Transfer Mini & Micro-channels: convective heat transfer in micro-channel with and without phase change, boiling and condensation in micro-channels, concepts and examples of micro heat exchange devices.

#### Text & Reference Books:

- 1. Tong, L. S., and Tang, Y. S., "Boiling Heat Transfer and Two-Phase Flow", 2<sup>nd</sup> Edition, Taylor& Francis 1997.
- 2. S. G. Kandlikar, "Handbook of Phase Change: Boiling and Condensation" Taylor & Francis, 1999.
- 3. Brennen, C. E., "Fundamental of Multi Phase Flow" Cambridge University Press, 2005.
- 4. Chang, L., and Mewes, D., "Advances in Multi Phase Flow and Heat Transfer", Bentham Science Publisher, 2009.

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# PROCESS INTENSIFICATION [CH-22403] [L:T:P:Cr = 4:0:0:4]

**Objective:** This course is aimed to provide the insights of compact, safe, energy-efficient and environment-friendly novel equipments and processes.

**Prerequisites:** Knowledge of basic chemical engineering courses particularly mass transfer, heat transfer and reaction engineering.

#### **COURSE OUTLINE**

Unit I [4 L]
Need of process intensification, process intensifying equipments and methods, examples of their application on
the commercial scale.
Unit II [10 L]
Use of high gravity fields, higee reactor, spinning disc reactors, micro-channel heat exchangers.
Unit III [10 L]
Monolithic catalyst and reactors, reverse flow reactor, micro-reactors.
Unit IV [10 L]
Concept and principle, reactive- distillation, extraction, precipitation adsorption, absorption, fermentation-
pervaporation, adsorptive distillation, membrane reactors and bioreactors.
Unit V [4 L]
Industrial practice (methodology, application) PI by improvement in existing plant and process synthesis, pi by
plants safety.

#### **Text/Reference Books:**

- 1. Stankiewicz, A.; Moulijn, J.A. "Re-engineering the chemical processing plant: process intensification" Marcel Dekker, Inc., New York, 2004.
- 2. Mizrahi, J. "Developing an industrial chemical process: an integrated approach" CRC Press, 2002.
- 3. Keil, F.J. "Modeling of Process Intensification" Wiley-VCH Verlag Germany, 2007
- 4. Reay, D.; Ramshaw, C.; Harvey, A. "Process Intensification" Elsvier, 2013
- 5. Boodhoo, K.; Harvey, A. "Process Intensification for Green Chemistry", Wiley, 2013.

#### PETROCHEMICAL TECHNOLOGY [CH-22404] [L:T:P:Cr = 4:0:0:4]

**Objective:** The course aims at providing information about processes leading to the manufacture of various petrochemical products.

Prerequisite: Basic knowledge about the sources of petrochemical products.

#### **COURSE OUTLINE**

#### Unit I

World and Indian petrochemicals scenario, petroleum refinery and petrochemical industries integration, manufacture of syngas from natural gas, chemicals based on direct reactions of methane: carbon disulfide, hydrogen cyanide, chloromethanes, chemicals based on synthesis gas: ammonia, methyl alcohol, ethylene glycol, steam pyrolysis of hydrocarbons (ethane, propane, naphtha), ethane chemicals, oxidation of propane, dehydrogenation of propane, nitration of propane, oxidation of n-butane.

#### Unit II

Oxidation of ethylene, derivatives of ethylene oxide, acetaldehyde, oxidative carbonylation of ethylene, vinyl chloride, perchloro and trichloroethylene, hydration of ethylene.

#### Unit III

Oxidation of propylene, disproportionation of propylene, alkylation using propylene, chlorination of propylene, hydration of propylene, properties and uses of isopropanol.

#### Unit IV

Alkylation of benzene, chlorination of benzene, nitration of benzene, oxidation of benzene, hydrogenation of benzene, dealkylation of toluene, oxidation of toluene, nitration of toluene, terephthalic acid, phthalic anhydride, isothalic acid.

#### Unit V

Polyethylene, polypropylene, poly vinyl chloride, polystyrene, nylon resins, polycarbonates, polyurethanes, epoxy resins, phenol-formaldehyde resins, butadiene polymers and copolymers, polyester fibres, polyamides, carbon fibres, polypropylene fibres.

#### **Text/Reference Books:**

- 1. Astle, M.J. "The Chemistry of Petrochemicals", Reinhold, 1956
- 2. Hatch, L.F; Matar, S. "From hydrocarbons to Petrochemicals", Gulf Pub. Co., 1981
- **3.** Matar, S.; Mirbach, M.J.; Tayim, H. A. "Catalysis in Petrochemical Processes", Kluwer Academic Publishers, 1989.
- **4.** Matar, S.; Hatch, L.F.; "Chemistry of Petrochemical Processes", Butterworth-Heinemann, 2<sup>nd</sup> Edition, 2001.
- 5. Steiner, H. "Introduction to Petroleum Chemicals", Pergamon Press, 1961.
- 6. Topchiev, A.V. "Synthetic Materials from Petroleum", Pergamon Press, 1962

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# NUCLEAR ENGINEERING [CH-22405] [L:T:P:Cr=4:0:0:4]

**Objective:** To acquaint students about the role of nuclear energy in the society at large and requisite information pertaining to nuclear reactors, nuclear fuels, and safe disposal of nuclear wastes.

#### **COURSE OUTLINE**

#### Unit I

Global and Indian nuclear energy scenario, nuclear energy based power plants in India, challenges associated with nuclear fuel supply, basics of nuclear physics, nuclear model of an atom, radio activity, half-life, neutron interactions.

# Unit II

Difference between nuclear fission and fusion, radio activity, chain reactions, critical mass and composition, nuclear fuel cycles and its characteristics, uranium, zirconium, thorium, beryllium production and purification.

# Unit III

Spent fuel reprocessing, spent fuel characteristics, nuclear fuel cycles, role of solvent extraction in reprocessing of spent fuel, Design of solvent extraction equipment.

# Unit IV

Various types of nuclear reactors in general, types of fast breeding reactors, design and construction of fast breeding reactors, fusion reactors, heat transfer techniques in nuclear reactors, reactor shielding.

# Unit V

Various aspects associated with safety and disposal of nuclear waste, types of waste, criteria for nuclear plant safety, safety systems, changes and consequences of accident, radiation hazards and their prevention.

# **Text/Reference Books:**

- 1. Lamarsh, J. R.; Baratta, A.J. "Introduction to Nuclear Engineering", Pearson, 2011.
- 2. Collier, J.G.; Hewitt, G.F. "Introduction to Nuclear power", Hemisphere Publishing, 1987.
- 3. El-Wakil, M.M. "Power Plant Technology", McGraw-Hill, 1984.
- 4. Bennet, D.J. "Elements of Nuclear Power", Prentice Hall Press, 1981.
- 5. Cannoly, T. J. "Fundamentals of Nuclear Engineering", John Wiley, 1978.

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# PROCESS SAFETY AND HAZARDS MANAGEMENT [CH-22406] [L: T: P: Cr = 4:0:0:4]

**Objective:** The aim of this course is to understand safety hazard and risk management related to chemical industries - preventing from losses, identifying the risk and solved the problem leading to hazards. **Prerequisites:** Basic knowledge on hazards and safety system of chemical industries.

#### **COURSE OUTLINE**

# Unit I

Introduction: The nature of hazards and risks, definition, relationship between hazards and risks in practice, a taxonomy of major chemical hazards, handing and storage of toxic chemicals, safety programs, accident and lost statics, significant of disasters.

# Unit II

Toxicology: Effects of toxicants on biological organisms, toxicological studies, dose versus response, relative toxicity, threshold limit values, industrial hygiene: government regulations.

#### Unit III

Fires and Explosions: Definition, the fire triangle, distinction between fire and explosion, the effect of dense explosives , flammability characteristics of liquids and vapours, VCE, over pressure, flash fire, pool fire, fire ball, jet fire, bleve, minimum oxygen concentration (MOC) and inerting, sprays and mists. toxic release and models: source models, dispersion models and pasquill-giffered models, release mitigation.

# Unit IV

Risk management, OHSA, ISO 14000, emergency response, Hazards identification: Process hazards checklist, hazard survey, QRA, HAZOP studies, fault tree and event tree, FMEA, LOPA, safety review, MSDS.

# Unit V

Introduction of reliefs: Concepts, definition, types of relief and relief sizing. safety in design and operation: safety in design, safety assurance in design, safety in operation, maintenance, organisation for safety, accident investigation and reporting.

# **Text/Reference Books**

- 1. Frank, P.L. "Loss Prevention in Process Industry", Butterworth Heinemann, London Vol. 1 & 2, 1996.
- 2. Roy, E.S. "Chemical Process Safety", Butterworth Heinemann, London, 3rd edition, 2005
- 3. Daniel A.C.; Louvar, J.F. "Chemical Process Safety Fundamental with Applications", Prentice Hall, New Jersey, 1990.
- 4. Marshall V.V. "Major Chemical Hazards", John Wiley and Sons, 1987.
- 5. Merv, F. "The Handbook of Hazardous Materials Spills Technology", McGraw-Hill, 2001.
- 6. Nicholas, P.C. "Handbook of Emergency Response to Toxic Chemical Releases", Noyes Publications, 1995.

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# FUNDAMENTALS OF BIOCHEMICAL ENGINEERING [CH-22407] [L:T:P:Cr = 4:0:0:4]

Objective: This course introduces the basic aspects of biochemical engineering and bioprocess technology and their commercial implications to the students from various disciplines. Prerequisites: UG level chemical engineering courses

#### **COURSE OUTLINE**

Unit-I [6 L]
Introduction to microbiology and biochemistry, classification and characteristics of microorganism, Essential
chemicals of life - lipids, sugars and polysaccharides, RNA and DNA, amino acids and proteins
Unit-II [12 L]
Enzymes and their classification, enzyme kinetics, immobilization of enzymes and whole cells, immobilized
enzyme kinetics
Unit-III [8 L]
Cell metabolism, regulation, stoichiometry, end products, cell growth kinetics, product formation kinetics,
thermal death kinetics, media and air sterilization
Unit-IV [6 L]
Transport phenomena in cellular systems, oxygen transfer rates, mass transfer coefficient and interfacial area,
mechanical agitation and power requirement
Unit-V [6 L]
Bioreactors: Type, design, operation and scale-up, instrumentation and control.
Down-stream processing, environmental concerns

#### **Text/Reference Books:**

- 1. Shuler M.L.; Kargi F. "Bioprocess Engineering: Basic Concepts" 2<sup>nd</sup> Ed., Prentice-Hall, 2003
- 2. Bailey, J.E.; Ollis, D.F. "Biochemical Engineering Fundamentals" 2<sup>nd</sup> Ed., McGraw Hill International Edition, 1987.
- 3. Blanch, H.W.; Clark, D.S. "Biochemical Engineering" Marcel Dekker, Inc., 1997.
- 4. Stanbury, P.F.; Whitaker, A. "Principles of fermentation technology" Pergamon Press, 1984.
- 5. Najafpour G. "Biochemical Engineering & Biotechnology", Elsevier, 2006.

# EXPERIMENTAL DESIGN AND DATA ANALYSIS [CH-22408] [L:T:P:Cr = 4:0:0:4]

**Objective:** The objective of this study is to help students develop a flair for research activity. This course will help them to design an experiment and understand logical way of data collection. **Prerequisites:** Knowledge of basic engineering mathematics.

# **COURSE OUTLINE**

Unit I [5 L]
Introduction, overview of subject, design of experiments and different approach to data analysis, introduction to
probability and statistics for chemical engineers.
Unit II [8 L]
Data analysis, fundamental, hypothesis test, comparison of mean and variance, correlation, analysis of variance,
interpretation of result, experimental data reporting.
Unit III [8 L]
Linear regression, least square methods, confidence interval constructions, model assessment.
Unit IV [8 L]
Experimental design principles, blocking, randomization, factorial design.
Unit V [8 L]
Variable selection, fractional factorial design, robustness, response surface methodology, individual factor and
interaction effects.

#### **Text/Reference Books**

- Montgomery D.C.; Runger G.C. "Applied Statistics and Probability for Engineers", 4th edition, John Wiley & Sons Inc, 2007
- 2. Mason R.L.; Gunst R.F.; Hess J.L. "Statistical Design and Analysis of Experiments with applications to engineering and science", 2nd edition, John Wiley & Sons Inc., 2005.
- 3. Lazic Z.R. "Design of Experiments in Chemical Engineering: A Practical Guide". John Wiley & Sons Inc, 2006.
- 4. Gonzalez. R. "Data Analysis for experimental design" Guilford Press. 2009.
- 5. Frigon N.L. "Practical Guide to experimental Design" JohnWiley & Sons. 1997.

# COLLOIDS AND INTERFACIAL ENGINEERING [CH-22409] [L:T:P:Cr = 4:0:0:4]

**Objective:** This course is aimed at introducing the basic concepts and tools for the analysis of colloidal and interfacial properties and their applications in adhesion, particle-aggregation, wetting, detergency, oil recovery, flotation, nucleation, bio-surfaces, chromatography, paints, composite materials. **Prerequisites:** Basic knowledge of physics and chemical engineering.

rerequisites: Basic knowledge of physics and chemical engineering

#### **Course Outline**

#### Unit I

Introduction, Surface Tension, Adhesion and Capillarity: effects of confinement and finite size, concepts of surface and interfacial energies and tensions, apolar (van der Waals) and polar (acid-base) components of interfacial tensions, Young-Laplace equation of capillarity; examples of equilibrium surfaces, multiplicity, etc. stability of equilibrium solutions, contact angle and Young's equation, determination of apolar (van der Waals) and acid-base components of surface/interfacial tensions, free energies of adhesion, kinetics of capillary and confined flows.

#### Unit II

Intermolecular, nanoscale and interfacial forces: Van der Waals, electrostatic double layer, acid-base interactions including hydrophobic attraction and hydration pressure.

# Unit III

Mesoscale thermodynamics, mesoscale phenomena in soft matter and applications: Gibbs treatment of interfaces, concept of excess concentration, variation of interfacial tensions with surfactant concentration, adhesion, wetting, nucleation, flotation, patterning of soft material by self - organization and other techniques.

# Unit IV

Stability of nanoparticle dispersions, nanofluidics: DLVO and DLVO like theories and kinetics of coagulation plus general principles of diffusion in a potential field/Brownian movement, stability of thin ( < 100 nm) films, self-organization in confined systems, meso-patterning.

# Unit V

Advanced and functional interfaces: Super-hydrophobicity, functional coatings, structural colors, nano-adhesives, nanocomposites.

# **Text/Reference Books**

1. Hiemenz, P.C. "Principles of Colloid and Surface Chemistry", Marcel Dekker, any edition starting with the 2nd edition, 1986.

2. Adamson, A.W. "Physical Chemistry of Surfaces" Wiley, 5th edition, 1990.

- 3. Hunter, R.J. "Foundations of Colloid Science", Clarendon, Oxford, Volume 1, 1989.
- 4. Russel, W.B.; Saville, D.A.; Schowalter, W.R. "Colloidal Dispersions", Cambridge University Press, 1989.
- 5. Israelachvili, J.N."Intermolecular and Surface Forces", Academic Press, 1992.
- 6. Oss, C. J.V. "Interfacial Forces in Aqueous Media", Marcel Dekker or Taylor & Francis, 1994.

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#### **CHARACTERIZATION OF MATERIALS [AM-22102]** [L:T:P:Cr = 4:0:0:4]

#### **COURSE OUTLINE**

#### **Crystallography:**

Bonding, Bravais lattices, Miller indices, symmetries in crystals, point groups, space groups, morphology, Crystal structures of common metal, ceramics, polymers. Imperfections in crystals, reciprocal lattice

#### X-ray Diffraction techniques:

Production of X-rays, its properties and hazards, Photon scattering, X-ray Diffraction and Bragg's law, Intensities calculations, Laue techniques, Debye-Scherrer techniques. Modern diffractometers, diffractometer measurements, Determination of crystal structure of powder sample, Small angle scattering, line broadening, particle size, crystallite size, residual stress measurement, Cell indexing, Precise parameter measurement, Phase identification, phase quantification, Phase diagram determination, stereographic projection, pole figure, Preferred orientation (Texture Analysis) and chemical analysis, Profile fitting and Rietveld analysis

#### **Optical microscopy:**

Principles and operations of microscopy, resolution, magnification, numerical aperture, depth of field, viewing area, contrast, Geometry of optical microscopes, application of microscopy in metallurgical studies (qualitative and quantitative), morphology and symmetry, grain boundaries and dislocation, phase contrast microscopy, polarised light microscopy, hot-stage microscopy, micro-hardness tester, sample preparation

#### **Electron microscopy:**

Electron diffraction, Principles and operation of scanning electron microscope. Geometry of electron microscopes, Electron Sources, Production of Vacuum, Pressure measurement, Leak detection, Specimen Handling and preparation, Secondary electron image, Backscattered electron image, Image processing, Analysis of electron micro-graphs and fractography studies. Transmission Electron Microscopy (TEM)

#### **Scanning Probe Microscopy:**

Principles and operation of scanning probe microscopes, Scanning Tunnelling Microscope, Atomic Force Microscope, Magnetic Force microscopy, Topography studies, Nano-indentation.

#### **Thermal Analysis:**

Thermo-Gravimetric Analysis, Differential Thermal Analysis, Differential Scanning Calorimetery, Thermo-Mechanical Analysis and their applications

#### Solid state and Surface spectroscopies:

Electron Energy Loss Spectroscopy (EELS), Reflection Absorption Infra-Red Spectroscopy (RAIRS), Transmission IR, Raman, Photoelectron, Spectroscopy (PES), Auger Electron Spectroscopy (AES), X-ray Fluorescence (XRF), Nuclear Magnetic Resonance (NMR), Extended X-ray Absorption Fine Structure (EXAFS).

#### **Term Paper:**

On application of techniques and/or on recent advances based on literature survey and/or lab/industry visit

#### **Text and references:**

1. Solid state chemistry and its Applications, Antony R. West, Wiley Student Edition

- 2. Elements of X-ray Diffraction, Cullity B. D., Addison-Wesley Publishing Co., 1979.
- 3. Electron Microscopy and Analysis, P.J. Goodhew, F.J. Humphreys, Taylor & francis, Second edition, 1997
- 4. Fundamentals of Molecular spectroscopy, Colin N. Banwell and Elaine M. McCash, Tat McGraw-Hill Publishing Co. Ltd., Fourth edition

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# PRINCIPLE OF BIOLOGICAL WASTEWATER TREATMENT [CE-22121] [L:T:P:Cr = 4:0:0:4]

#### **Course Outline**

Unit I: [6L]
Wastewater characterization: Analysis of BOD, COD and other parameters
Unit II: [8L]
Unit Operations, Reaction kinetics, Types of reactors and reactor dynamics, Analysis of ideal and field reactors
Unit III: [6L]
Bio-kinetic parameters and their evaluation, Biomass yield, Cell maintenance, Energy considerations
Unit IV: [8L]
Principles of oxidation in stabilization ponds, ASP, Trickling filter, Aerated lagoons and RBCs. Principle of
aerobic and anaerobic processes and design considerations, Design model and equations, Principles of
nitrification de nitrification and anoxic processes.
Unit V: [6L]
Mass Transfer, Diffusion and attached growth processes.
Unit VI: [6L]
Principles of sludge stabilization and chemical oxidation, Principle and design of sludge digestion

#### References

- 1. Metcalf and Eddy, Inc. ""Wastewater Engineering-Treatment, Disposal and Reuse", 7th edition, Tata McGraw-Hill Publishing Company Limited, New Delhi, 2007.
- 2. Weber, "Physico-chemical Processes for Water Quality Control"
- 3. Peavy, H.S., Rowe, D.R. and Tchobanohous, G. Enviormental Engineering", McGraw-Hill Book Co., International Ed., 1985.
- 4. Fair, Geyer and Okun, "Waste Water Engineering, Vol- I and II
- 5. Arceivala, S.J. (2002), "Wastewater Treatment for Pollution Control", 2nd Ed., Tata McGraw-Hill, New Delhi.
- 6. Gray, N.F. (2000)."Water Technology"1st Indian Ed., Viva Books, New Delhi.

# ENVIRONMENTAL IMPACT ASSESSMENT [CE-22358] [L:T:P:Cr = 4:0:0:4]

#### **Course Outline**

Unit I : [6L] Overview of EIA; EIA at different level: Regional; policy; sector levels, EIA process; Screening and scoping criteria
Unit II: [8L]
Rapid and comprehensive EIA; Legal and Regulatory aspect in India; Environmental risk analysis; Economic valuation methods; Cost-benefit analysis; expert system and GIS applications; Uncertainties
Unit III: [8L]
Legislative and environmental clearance procedures in India and other countries, siting criteria; CRZ; Public participation; Resettlement and rehabilitation plans.
Unit IV: [6L]
Practical applications of EIA; EIA methodologies; Baseline data collection; Predication and assessment of
impacts on physical, biological and socio economic environment
Unit V: [6L]
Environmental management plan; Post project monitoring, Environmental audit, EIA Report and EIS; Review
Processes
Unit VI: [6L]
Case studies on EIA projects and Environmental Management Plan
Reference Books:

- 1. Canter, L.W., Environmental Impact Assessment", McGraw Hill, New York, 1996.
- 2. Petts, J., "Handbook of Environmental Impact Assessment Vol I and II", Blackwell Science, London, 1999.
- 3. The World Bank Group, Environmental Assessment Sourcebook Vol I, II and III", The World Bank, Washington, 1991.
- 4. Waddams, L. "Chemicals from Petroleum", Chemical publishing, 1969.