# **CURRICULUM AND SYLLABI**

# M.Tech

# in

# **CHEMICAL ENGINEERING**

(With effect from Academic Year 2018-2019)



# DEPARTMENT OF CHEMICAL ENGINEERING NATIONAL INSTITUTE OF TECHNOLOGY CALICUT KERALA- INDIA -673601

# **Programme Educational Objectives (PEO)**

To train students to be highly-skilled professionals in chemical engineering and
allied fields who can successfully analyse and solve complex chemical engineering
problems
To enable graduates to carry out and disseminate innovative research work in
academia / industry to enhance the knowledge base in chemical engineering.
To prepare the post-graduates professionals in chemical engineering of integrity,
social responsibility and life-long independent learning ability.
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# **Programme Outcomes**

PO1	Attain abilities to identify, formulate and solve problems under chemical engineering purview
PO2	Acquire capacity to devise and conduct experiments, interpret data and provide well informed conclusions
PO3	Be able to work effectively in interdisciplinary teams to develop efficient systems for the industry and society
PO4	Be able to conduct independent research and generate new knowledge for the benefit of mankind
PO5	Be able to use modern engineering tools, software and equipment to analyse various problems in chemical industry
PO6	Be able to effectively communicate through technical reports, presentations and scientific publications with the engineering community as well as society at large
PO7	Develop ability for self-education and life-long learning
PO8	Be able to maintain a high level of professional and intellectual integrity, ethics of research and scholarly standards

	CORE SUBJECTS					
	Semester 1					
Code	Name of the Subject	L	Т	P/S	С	
	Communicative English (audit only)	3	0	0	0	
MA6001D	Mathematical Methods for Engineers	3	0	1	3	
CH6002D	Chemical Engineering Thermodynamics	3	0	0	3	
CH6003D	Momentum, Heat and Mass Transfer	3	0	0	3	
CH6004D	Process Modeling and Simulation	3	0	0	3	
CH6091D	Analytical and Instrumentation Techniques in Chemical Engineering Laboratory	0	0	3	2	
	Elective 1	3	0	0	3	
Total Credi	ts			1	17	

Semester 2					
Code	Name of the Subject	L	Т	P/S	С
CH6005D	Chemical and Catalytic Reaction Engineering	3	0	0	3
CH6006D	Optimization for Chemical Engineers	3	0	0	3
CH6007D	Advanced Separation Processes	3	0	0	3
CH6008D	Chemical Process Control	3	1	0	3
CH6092D	Seminar	0	0	2	1
CH6093D	Computer Applications in Chemical Engineering Laboratory	0	0	3	2
	Elective 2	3	0	0	3
Total Credit	s	•	•	•	18

Semester 3							
Code	Name of the Subject	L	T	Р	С		
CH7001D	Project Work – Part 1	0	0	40	10		

Semester 4							
Code	Name of the Subject	L	T	Р	С		
CH7002D	Project Work – Pat 2	0	0	60	15		

Total Number of Credits – 60, # Core courses – 8 # Elective Courses – 2, (Soft Core courses – Nil)

LIST OF ELECTIVE COURSES						
Code	Name of the Subject	L	T	P/ S	С	
CH6021D	Advanced Computational Fluid Dynamics	3	0	0	3	
CH6022D	Bioprocess Engineering	3	0	0	3	
CH6023D	Fluidization Engineering	3	0	0	3	
CH6024D	Environmental Engineering	3	0	0	3	
CH6025D	Biological Wastewater Treatment	3	0	0	3	
CH6026D	Bioreactor Engineering	3	0	0	3	
CH6027D	Safety Management in Process Industries	3	0	0	3	
CH6028D	Fire Engineering and Explosion Control	3	0	0	3	
CH6029D	Fire Modeling and Dynamics	3	0	0	3	
CH6030D	Advanced Polymer Technology	3	0	0	3	
CH6031D	Multiphase Systems and Reactors	3	0	0	3	
CH6032D	Advanced Transport Phenomena	3	0	0	3	
CH6033D	Numerical Methods in Chemical Engineering	3	0	0	3	

# Notes:

- 1. A minimum of 60 credits have to be earned for the award of M. Tech Degree in this Programme.
- 2. Communicative English and Audit courses are optional. Industrial Training during summer is optional.
- 3. # Core courses 8; # Elective Courses 2 (Soft Core courses Nil)

# MA6001D MATHEMATICAL METHODS FOR ENGINEERS

Pre-requisites: Nil Total hours: 39

L	Т	Р	C
3	1	0	3

#### **Course Outcomes:**

- CO1: Learn Vector spaces, Inner product spaces, Linear transformations and construct orthonormal basis.
- CO2: Find power series solutions of ODEs, study Legendre, Bessel equations, learn Frobenius method and Sturm-Liouville problem.
- CO3: Use Lagrange method, Charpit's method, Jacobi method to find the solution of first order PDEs and use method of separation of variables to solve linear second order PDEs.
- CO4: Learn coordinate transformations, covariant, contravariant and mixed tensors, conjugate tensor, Quotient law, Christoffel's symbols and covariant derivative.

# Module: I (10 Hours)

Linear Algebra: Vector spaces, Subspaces, Basis, Dimension, Inner product spaces, Gram-Schmidth Process, Linear Transformations, Range and Kernel, Isomorphism, Matrix of transformations and Change of Basis.

#### Module: II (9 Hours)

Series Solutions of ODE and Sturm-Liouville Theory: Power series solutions about ordinary point, Legendre equation and Legendre polynomials, Solutions about singular points; The method of Frobenius, Bessel equation and Bessel Functions. Sturm-Liouville problem and Generalized Fourier series.

# Module: III (10 Hours)

Partial Differential Equations: First order PDEs, Linear equations, Lagrange method, Cauchy method, Charpits method, Jacobi method. Second order PDEs, Classification, Method of separation of variables, Formulation and solution of Wave equation, Heat equation and Laplace equation.

# Module: IV 10 Hours)

Tensor Calculus: Spaces of N-dimensions, coordinate transformations, covariant, contravariant and mixed tensors, fundamental operation with tensors, Quotient Law, The line element and metric tensor, conjugate tensor, Christoffel's symbols, covariant derivative.

- 1. D. C. Lay: Linear Algebra and its Applications, Addision Wesley, 2003.
- 2. F. G. Florey: Elementary Linear Algebra with Application, Prentice Englewood, 1979.
- 3. W. W. Bell: Special Functions for Scientists and Engineers, Dover Publications, 2004.
- 4. Ian Sneddon, Elements of Partial Differential Equations, McGraw Hill International, 1985.
- 5. B. Spain: Tensor Calculus, Oliver and Boyd,1965.
- 6. K.SankaraRao,Introduction to Partial Differential Equations,Prentice-Hall of India Pvt.Ltd; 3 edition, 2010.
- 7. Shepley L Ross, Differential Equations, JohnWiley&Sons, Third Edition, 2004.
- 8. L.A.Pipes and L.R. Harwill: Applied Mathematics for Engineers and Physicists, McGraw Hill, 1971.
- 9. M.A. Akivis and V.V Goldberg, An Introduction to Linear Algebra and Tensors, Dover Publications,1997.
- 10. Prasun Kumar NayakText book, of Tensor Calculus and Differential Geomatry,PHI Learning Pvt. Ltd New Delhi, 2012.

#### CH6002D CHEMICAL ENGINEERING THERMODYNAMICS

L	Т	Р	C
3	0	0	3

Pre-requisites: Nil Total hours: 39

#### Course outcomes:

CO1: Measurement of interactions and surface forces, electrostatic interactions, modeling interaction potential functions.

CO2: Microstates of the system under the same macroscopic condition or having the same microstate- illustrate the case of a gas that has N identical diatomic molecules- probability distribution over possible -Quantum states

CO3: Dynamics of a multicomponent gas mixture in states close to local equilibrium

CO4: Entropy, its flow and production - consideration on the disturbance from the surroundings conventional and non-conventional type reciprocity

# Module 1 (13 hours)

Statistical Thermodynamics: Ensemble; Most probable distribution; Canonical, grand canonical and micro-canonical ensemble partition functions; Derivation of thermodynamic variables from partition functions; Statistical explanation of second and third laws of thermodynamics; Quantum statistics; Applications of Maxwell Boltzmann, Fermi-Dirac, and Bose-Einstein Staistics; Thermodynamic properties of perfect gas; Einstein and Debye theory of crystalline solids; Langmuir and BET isotherms of adsorption of gas on lattice structure.

# Module 2 (14 hours)

Non-equilibrium thermodynamics: Maxwell distribution; Mean free path and collision frequency; Introductory transport theory; Boltzmann transport equation; Two particle collisions; Boltzmann H theorem; Conservation laws; Zero order approximation and its application; First order approximation and applications; Introduction to Chapman-Enskog approximation of distribution function

#### Module 3 (12 hours)

Irreversible thermodynamics: Conjugate fluxes and driving forces; Onsager reciprocal relation; Simultaneous heat and mass transfer problems; Multi-component mass transfer problems; Heat transfer in anisotropic media; Formulation of the problem for a single reaction; Affinity of a reaction; Application in more than one reactions

- 1.S.I. Sandler, Chemical, Biochemical and Engineering Thermodynamics, 4th Ed.., Wiley Publications, 2006.
- 2. J.M Smith,. H.C. Van Ness, M.M. Abbott, Introduction to Chemical Engineering Thermodynamics, 6th ed Mc Graw Hill Publications, 2005
- 3. D Denbigh, Kenneth. Principles of Chemical Equilibrium. 4 th Ed., Cambridge University Press, 1981.
- 4. Dr David Tong, Statistical Physics, University of Cambridge Part II Mathematical Tripos, 2012
- 5. Keith Stowe, An Introduction to Thermodynamics and Statistical Mechanics, Second Edition, 2007

# CH6003D MOMENTUM, HEAT AND MASS TRANSFER

Pre-requisites: Nil Total hours: 39 Course Outcomes:

L	Т	Р	С
3	0	0	3

CO1: Derivation of momentum and energy balance equations

CO2: Write the basic heat transfer equations

CO3: Solve problems based on momentum balance

CO4: Write mass balance equations

CO5: Derive the balance equations for any process given and derive dimensionless numbers

# Module 1 (13 hours)

Introduction to Transport Processes, Basic Mass, Momentum, and Energy transport processes; micro and macroscopic views; phenomenological laws; driving forces; transport coefficients. Definition of fluxes; conservation principles; differential elementary volumes and coordinate systems; boundary conditions; dimensionless numbers. Molecular mass transport – Fick's law of binary diffusion; binary gaseous diffusion coefficient – kinetic theory; diffusion in liquids and solids. Effective transport properties (diffusion in suspensions and through a pack of spheres) Steady and transient diffusion processes

# Module 2 (16 hours)

Momentum Transport and Viscous Flows. Newton's law of viscosity; molecular theory of viscosity of dilute gases and liquids; Couette and falling film flow; momentum as a flux and as a force – viscous stress tensor; Shell momentum balance and laminar flows – principles; Poiseuille flow; flow in an annulus; creeping flow around a sphere. Continuity and equations of change, Navier-Stokes equations. Macroscopic balances for momentum transport Turbulent flows, Reynolds experiment, drag forces; turbulence and eddy flow (similarities with molecular transport) and atmospheric fluxes (eddy covariance method). Energy Transport – Fourier's law of heat conduction; thermal conductivity - molecular and effective; heat flow in one and multi-dimensional geometries; steady-state and transient analytical solutions to heat conduction; heat flow and convection; nonlinear cooling, macroscopic energy balance. Radiative energy transport – Stefan-Boltzmann law; black body exchange, principles, and examples

#### Module 3 (10 hours)

Phase change and couple heat and mass transport (falling film, evaporating water drop) Mass Transport in Solid and in Laminar Flow: Shell mass balances: boundary conditions, diffusion through a stagnant gas film, diffusion with heterogeneous chemical reaction, diffusion with homogeneous chemical reaction, diffusion into a falling liquid film I forced – convection mass transfer, diffusion and chemical reaction inside a porous catalyst: the "effectiveness factor". Analogies between heat, mass and momentum and transfer.

- 1. Bird R B, Stewart W E and Light fort R N, "Transport Phenomena", John Wiley and Sons (2002).
- 2. Welty JR, Wilson RE and Wicks C E, "Fundamentals of Momentum, Heat, and Mass Transfer", 4th ed, John Wiley and Sons (2001).
- 3. John C Slattery, "Momentum, Energy and Mass transfer in continua", McGraw Hill, Co. (1972).
- 4. Bennet C U and Myers J E, "Momentum, Heat, and Mass Transfer" Tata McGraw Hill Publishing Co. (1975)
- 5. Robert S Brodkey and Harry C Hersing, "Transport Phenomena a Unified approach" McGraw Hill Book Co. (1988)

# CH6004D PROCESS MODELING AND SIMULATION

L	T	Р	С
3	0	0	3

Pre-requisites: Nil Total hours: 39 Course outcomes:

- CO1: Demonstrate the applications of process modeling and simulation in chemical engineering, its usefulness, and limitations
- CO2: Build various chemical engineering process models based on fundamental laws
- CO3: Develop skills for the numerical solution of process models
- CO4: Model and solve various real-life chemical engineering process using MATLAB and interpret simulation results
- CO5: Distinguish between process modeling and process flow sheeting and explain various solution approaches to process flow sheeting

# Module 1: (15 hours)

Introduction to process modeling and simulation, its usefulness, and limitations, classification of models, mathematical complexity and scale, fundamental laws on which models are built-conservation laws; chemical reaction engineering; thermodynamics; transport phenomena; equations of state; equilibrium, model building, types of variables and degrees of freedom analysis. Development of isothermal and non-isothermal models for various process units- stirred tank; jacketed vessel; surge tank; heat exchangers, packed column; reactors, mixing tank; absorption column; multi-component flash drum and distillation column, Linearization of models, state space models, system stability.

# Module 2: (12 hours)

Solution techniques for steady state and unsteady state lumped parameter models which leads to algebraic and ordinary differential equations (initial value problems) - explicit Euler method; implicit Euler method; Runge-Kutta methods; Solution techniques for steady state and unsteady state distributed parameter models which leads to ordinary differential equations (initial value problems and boundary value problems with Dirichlet, Neumann and Robin and mixed boundary conditions), and partial differential equations (implicit and explicit method, Crank-Nicolson method), Introduction to MATLAB.

# Module 3: (12 hours)

Simulation of the process models for various units of plant and operations using MATLAB, step-size strategies, convergence criteria, analysis and interpretation of simulation results, process flowsheeting, physical property service facilities, degrees of freedom in a flow sheet, sequential modular, simultaneous modular and equation-oriented approaches to flow sheeting, partitioning and tearing of streams, tearing algorithms.

- B.W. Bequette, Process Dynamics: Modeling, Analysis and Simulation, New Jersey, Academic press, 2001
- 2. William L. Luyben, Process Modeling, Simulation and Control for Chemical Engineers, 2<sup>nd</sup> ed. McGraw-Hill Publishing Company, New York, 1999
- 3. B. Ogunnaike and W. Haemon Ray Process Dynamics, Modeling and Control, Oxford University Press Oxford, 2006
- 4. Hussain Chemical Process Simulation, Wiley & Sons, INC. New York, 1986
- 5. S.C. Chapra and R.P. Canale, Numerical Methods for Engineers, 7<sup>th</sup>ed McGraw-Hill Education NewYork, 2015
- 6. R.G.E Franks, Modeling, and Simulation in Chemical Engineering, John Wiley, 1972.
- 7. A.W. Westerberg, H.P. Hutchison, R.L. Motard, P. Winter, Process Flowsheeting, Cambridge University Press Cambridge 1979

# CH6091D ANALYTICAL AND INSTRUMENTATION TECHNIQUES IN CHEMICAL ENGINEERING LABORATORY

Pre-requisites: Nil Total hours: 27

L	Т	Р	С
0	0	3	2

#### Course outcomes:

- CO1: Understand the theoretical principles, instrumentation and applications of various analytical instruments
- CO2: Determine the physical, chemical and mechanical properties of substance using sophisticated instruments
- CO3: Analyse the chemicals using spectrometry and chromatography methods
- CO4: Execute qualitative and quantitative analysis of chemical species using thermal and electrochemical methods.
- Determination of concentration of an unknown sample using spectrometry instruments like Atomic absorption, UV-Visible spectrophotometers.
- Identification of the functional groups present in the given samples using Fourier transform infrared spectroscopy.
- Testing the mechanical strength of the given material using universal testing machine and analyze the properties of the material using BET Surface area analyzer.
- Quantitative analysis by Gas Chromatography and High performance liquid chromatography.
- Electrochemical method of chemical analysis.
- Characterization of materials using Thermo gravimetric analyzer.

#### List of Equipments/Techniques

- 1. Absorption spectroscopy (atomic absorption, UV-Visible)
- 2. Vibrational spectroscopy (Infrared spectrophotometer)
- 3. Flame photometer
- 4. Gas chromatograph
- 5. High-performance liquid chromatography
- 6. Ion chromatography
- 7. Thermogravimetric analyzer
- 8. Differential scanning calorimeter
- 9. Differential thermal analyzer
- 10. BET surface area analyzer
- 11. Universal Testing Machine
- 12. Electrochemical analysis (polarography, pulse polarographic methods, anodic stripping voltammetry)
- 13. Conductivity meter
- 14. Optical microscope

- 1. R S Khandpur : Handbook of Analytical Instruments, McGraw Hill Education (India) Pvt. Ltd publications, Third edition, 2015.
- 2. Francis Rouessac and Annick Rouessac :Chemical Analysis: Modern Instrumentation Methods and Techniques, Wiley publishers, Second edition, 2005.

# CH6005D CHEMICAL AND CATALYTIC REACTION ENGINEERING

Pre-requisites: Nil Total hours: 39

10	Τ	Р	O
3	0	0	3

#### **Course outcomes:**

CO1: Analyze non catalytic and catalytic reactions.

CO2: Develop the knowledge of catalyst preparation and characterization.

CO3: Design of experiments involving physical adsorption and chemical adsorption, analyzing and interpreting data.

CO4: Design and stability analysis of different reactors on the basis of kinetic data obtained.

#### Module 1 (15 hours)

Analysis of Noncatalytic fluid-solid reaction: Kinetics of non-catalytic fluid-particle reactions, various models, application to design. Catalyst preparation and characterization: Catalysis - Nature of catalysis, methods of evaluation of catalysis, factors affecting the choice of catalysts, promoters, inhibitors, and supports, catalyst specifications, preparation and characterization of catalysts, surface area measurement by BET method, pore size distribution, catalyst, poison, mechanism and kinetics of catalyst, deactivation.

#### Module 2 (12 hours)

Physical adsorption and chemical adsorption: Fluid-fluid reactions different regimes, identification reaction regime, application to design. Physical absorption with chemical reaction, simultaneous absorption of two reacting cases consecutive reversible reactions between gas and liquid, irreversible reactions, estimation of the effective interfacial area in absorption equipment.

#### Module 3 (12 hours)

Reaction kinetics, accounting porous nature of catalyst: Heterogeneous catalytic reactions - effectiveness factor, internal and external transport processes, non-isothermal reacting systems, uniqueness and multiplicity of steady states, stability analysis. Modeling of chemical reactors: Modeling of multiphase reactors - Fixed, fluidized, trickle bed, and slurry reactors.

- 1. G.F. Froment, K.B. Bischoff, Chemical Reactor Analysis and Design, 2nd Ed., John Wiley, New York, 1990.
- 2. O. Levenspiel, Chemical Reaction Engineering, 3rd Ed., Wiley Singapore, 2000.
- 3. J.J. Carberry, Chemical and Catalytic Reaction Engineering, McGraw Hill, New York, 2001.
- 4. R. Aris, Elementary Chemical Reactor Analysis, Prentice Hall, 1989.
- 5. H. Scott Fogler, Elements of Chemical Reaction Engineering, 5th Ed, Prentice Hal, 2016

# **CH6006D OPTIMIZATION FOR CHEMICAL ENGINEERS**

L	Т	Р	С
3	0	0	3

Pre-requisites: Nil Total hours: 39

#### **Course Outcomes:**

CO1: Develop in depth knowledge of traditional optimization techniques

CO2: Apply more advanced optimization techniques like genetic algorithms and differential evolution

CO2: Carry out optimization problems for optimum design and production of products for real largescale process plant

# Module 1: (12 hours)

Functions of single and multiple variables: optimality criteria, direct and indirect search methods. Nonlinear Programming: Lagrange multipliers, Kuhn-Tucker conditions, first-order and second-order optimality conditions, Transformation methods based on linearization: penalty concept, various penalty terms, and method of multipliers

# Module 2: (12 hours)

Quadratic Programming: quadratic approximation methods for constrained problems, applications of quadratic programming. Geometric Programming: geometric programming modeling approach, applications of geometric programming. Optimality criteria and optimal control Problems: Euler-Lagrange optimality criteria, Pontryagin's maximum principle, optimal control problems.

# Module 3: (15 hours)

Dynamic programming, mixed Integer linear programming, mixed Integer nonlinear programming. Non Traditional optimization techniques: Simulated annealing, Genetic algorithms, and differential evolution. Application of optimization in the design of separation process, chemical reactor, and large-scale process plant.

- 1.T.F. Edgar and D.M. Himmelblau, Optimization of Chemical Processes, 2<sup>nd</sup> ed., New York: McGraw-Hill, 2001.
- 2.A. Ravindran, K.M. Ragsdell, and G.V. Reklaitis, Engineering Optimization, 2<sup>nd</sup> ed., New Jersey: John Wiley & Sons, 2006.
- 3. R. Smith, Chemical Process Design, and Integration, New Jersey: John Wiley & Sons Ltd, 2005.
- 4. G. G. Luenberger and Y. Ye, Linear and Nonlinear Programming, 3<sup>rd</sup> ed., New York: Springer, 2008.
- 5. S.S. Rao, Engineering optimization Theory and Practice, 4<sup>th</sup> ed., New Jersey: John Wiley & Sons, 2009.
- 6. K.Deb, optimization for engineering design: Algorithms and examples, Prentice-Hall of India, New Delhi 2002

# **CH6007D ADVANCED SEPARATION PROCESSES**

Pre-requisites: Nil Total hours: 39

# Course Outcomes:

L	Т	Р	O
0	3	0	3

CO1: Identify various conventional and modern separation techniques in chemical engineering processes

CO2: Describe the fundamentals of membrane separation and charged based separation techniques

CO3: Analyze conventional and advanced extraction and filtration systems

CO4: Apply the knowledge of surface and ionic properties in the separation process

CO5: Analyze and design different membrane modules, chromatographic and ion exchange systems for intended applications

# Module 1 (13 hours)

General: Review of conventional processes., Membrane separations: Types and choice of membrane, plate and frame tubular spiral wound and hollow fibre membrane reactors and their relative merits, commercial pilot plant and laboratory membrane permeators involving dialysis, reverse osmosis, nanofiltration, ultrafiltration, microfiltration and Donnan dialysis, economics of membrane operators, ceramic membranes. pervaporation and permeation techniques for solids liquids and gases

# Module 2 (13 hours)

Recent advances in separation techniques based on size surface properties, ionic properties and other special characteristics of substances, process concept theory, and equipment used in crossflow filtration, cross-flow electro filtrations, Separation by adsorption Techniques and Ionic separations: Mechanism types and choice of adsorbents, normal adsorption techniques, affinity chromatography and immune chromatography,

# Module 3 (13 hours)

Types of equipment and commercial processes, recent advances and process economics, controlling factors, applications, types of equipment employed for electrophoresis, dielectrophoresis, ion exchange chromatography and electrodialysis, commercial processes, Other Techniques: Separation involving lyophilisation, industrial viability and examples, zone melting, adductive crystallization, other separation processes, supercritical fluid extraction, oil spill management, industrial effluent treatment by modern techniques- dual function filter surface based solid-liquid separations involving a second liquid sirofloc filter.

- 1. King, C.J., Separation Processes, Tata Mc Graw Hill Co. Ltd., 1982.
- 2. Hanson, C., Baird, M.H.I. and T.C., Hand Book of Solvent Extraction, Wiley International, New York, 1983.
- 3. Nakagawal, O.V., Yoshihito Osada., Membrane Science and Technology, Marcel Dekker, 1992.
- 4. Lacey, R.E. and Looeb, S., Industrial Processing with membrane, Wiley Inter-Science New York, 1972.
- 5. Schoen, H.M., New Chemical Engineering Separation Techniques, Wilev-Inter Science, 1972.
- 6. Rousseau, R.W., Hand Book of Separation Process Technology, John Wiley, New York, 1987.

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# CH6008D CHEMICAL PROCESS CONTROL

Pre-requisite: Nil Total hours: 39

L	Т	Р	С
3	1	0	3

#### **Course Outcomes:**

CO1: Knowledge of different control strategies used in the chemical industry

CO2: Tuning and decoupling of controllers in MIMO systems

CO3: Thorough knowledge of the application of modeling and simulation tools for the control of chemical processes

CO4: Understanding and implementation of advanced control strategies for chemical processes

# Module 1 (13 hours)

Review of process control topics, cascade control, Split-range control, Override control, Valve position control, Ratio and feedforward control, Loop interaction, decoupling.

# Module 2 (13 hours)

Process identification techniques for SISO and MIMO systems, generalized predictive control, Model predictive control, Dynamic Matrix Control

# Module 3 (13 hours)

Multivariable control, internal mode control, optimal control, control structure design for complete chemical plants, case studies using process engineering packages.

- 1.M. L. Luyben, W.L. Luyben, Essentials of Process Control, Mc-Graw Hill, 1997.
- 2.C. L. Smith, Advanced Process Control, Beyond Single Loop Control, Wiley, 2010.
- 3.B. A. Ogunnaike, W. H. Ray, Process Dynamics, Modeling, and Control, Oxford University Process, 1994.
- 4.W. L.Luyben, Plantwide Process Control, McGraw-Hill, 1999.

# **CH6092D SEMINAR**

L	Т	Р	С
0	0	2	1

Pre-requisite: Nil

CO1: Demonstration of the presentation skills in real-time environment

CO2: Thorough understanding of technical resources towards successful preparation for a talk/lecture

CO3: Preparation of oral presentations related to the technical assignments

Each student shall prepare a paper on any topic of interest in the field of Chemical Engineering. He/she shall get the paper approved by the Program Coordinator/Faculty Advisor/Faculty Members in the concerned area of specialization and present it in the class in the presence of Faculty-in-charge of seminar class. Every student shall participate in the seminar. Grade will be awarded on the basis of the student's paper, presentation and his/her participation in the seminar.

# CH6093D COMPUTER APPLICATIONS IN CHEMICAL ENGINEERING LABORATORY

Pre-requisites: Nil Total hours: 27

L	Т	Р	С
0	0	3	2

#### Course outcomes:

CO1: Develop MATLAB programming skills

CO2: Solve chemical engineering problems using MATLAB

CO3: Develop skills to carry out process simulation in Aspen HYSYS

CO4: Solve simple and complex flowsheets in Aspen HYSIS

MATLAB programming: Syntax of MATLAB programming, plotting and graphics handling, file handling, writing user-defined functions, use of inbuilt functions, symbolic math, introduction to Simulink, programs to solve problems in chemical engineering- thermodynamics; transport phenomena; reaction engineering. Aspen HYSYS Simulation: Setting up problems in Aspen Plus and Aspen Hysys, simulation of individual equipment/operation, creating user-defined models, property analysis and estimation using Aspen property package, simulation of equilibrium staged operations, simple and complex flow sheets, performing sensitivity analysis, and design calculation, analysis of properties of pure components, binary mixtures and mixtures, process and mechanical design of shell and tube heat exchanger, analysis of pipeline hydrolysis

- 1. S.C. Chapra and R.P. Canale, Numerical Methods for Engineers, 7<sup>th</sup> ed McGraw-Hill Education New York, 2015
- 2. R.R. Kapuno, Programming for Chemical Engineers using C, C++ and MATLAB, Hingham, Mass, Infinity Science, 2008
- 3. A.W. Westerberg, H.P. Hutchison, R.L. Motard, P. Winter, Process Flowsheeting, Cambridge University Press Cambridge 1979

# CH7001D PROJECT WORK - PART 1

L	Т	Р	С
0	0	40	10

**Pre-requisite:** A student should have registered for all theory and laboratory courses in the first and second semester of the programme and secured a grade other than 'W''

#### **Course Objectives:**

CO1: Identify and formulate the problem in the selected topic and arrive at a suitable solution.

CO2: Demonstrate and generate new knowledge of their selected project topic.

CO3: Able to communicate with the industry, academia or society at large in written and oral forms

The project work starts in the third semester and extends to the end of the fourth semester. The student will be encouraged to fix the area of work and conduct the literature review during the second semester itself. The topic shall be research and development oriented. The project can be carried out at the institute or in an industry/research organization. Students desirous of carrying out the project in industry or other organization have to fulfill the requirements as specified in the "Ordinances and Regulations for Master of Technology (M.Tech.) Programme Under the section - Project Work in Industry or Other Organization. "At the end of the third semester, the students' thesis work shall be assessed by a committee and graded as specified in the "Ordinances and Regulations for Master of Technology (M. Tech.) Programme". If the work has been graded as unsatisfactory, in the third semester the committee may recommend a suitable period by which the project will have to be extended beyond the fourth semester.

# CH7002D PROJECT WORK - PART 2

L	Т	Р	C
0	0	60	15

# **Course Objectives:**

CO1: Design and execute the project individually

CO2: Apply the solution approach to the other similar kind in the chemical engineering domain

CO3: Able to conduct in professional way as successful post-graduate engineer

At the end of the fourth semester, the student shall present his/her thesis work before an evaluation committee, which will evaluate the work and decide whether the student may be allowed to submit the thesis or whether he/she needs to carry out additional work. The final viva-voce examination will be conducted as per the "Ordinances and Regulations for Master of Technology (M. Tech.) Programme"

# CH6021D ADVANCED COMPUTATIONAL FLUID DYNAMICS

Prerequisite: Nil Total hours: 39

L	Т	Р	С
3	0	0	3

#### **Course outcomes:**

CO1: Derive the governing equations for fluid flow

CO2: Apply finite difference and finite volume methods to fluid flow problems

CO3: Calculate and solve a heat transfer problem

# Module 1 (14 hours)

Introduction to Computational Modeling of Flows -significance with a special emphasis on chemical engineering applications. – Index notation of vectors and tensors-Control volume-Reynolds Transport Theorem-Governing equations- Non-dimensional forms-Phenomenological models-boundary conditions-classification, detailed study of Navier Stokes equation- Solution of the Navier Stokes equations

# Module 2 (13 hours)

Turbulence Modelling -The Turbulence Problem-Algebraic and Differential Models, k-models, other models. Numerical methods for CFD-classification of PDE's-Basic discretization methods- Mesh-solution, and convergence iterative methods-Properties of numerical solutions-accuracy and errors-Application of numerical methods to selected model equations such as wave equations-heat equation. Laplace's equation-Burgers equation-First and Second order methods - upwind, Lax Wendroff, McCormack methods etc.

#### Module 3 (12 hours)

Finite Volume Method - Discretization of convective, viscous, pressure and body force terms-conservation properties-grid arrangement-collocated, staggered-pressure equation, and its solutions-implicit and explicit methods-implicit pressure correction methods-Fractional Step method SIMPLE algorithm for a collocated Variable arrangement.

- 1. H. K. Versteeg and W. Malalasekera, An introduction to computational fluid dynamics: the finite volume method, Longman scientific & technical publishers, 2007
- 2. D.A. Anderson, J.C. Tanneheil, R. H. Pletcher, Computational Fluid Mechanics and Heat Transfer, Hemispher, New York, 1984
- 3. G.D. Smith, Numerical Solution of Partial Differential Equations: Finite Difference Methods, Calderon Press, Oxford
- 4. V. PatankarSuhas, Numerical Heat Transfer and Fluid Flow, McGraw Hill, Washington, 1980.

#### **CH6022D BIOPROCESS ENGINEERING**

Pre-requisites: Nil Total hours: 39

L	Т	Р	С
3	0	0	3

#### **Course Outcomes:**

CO1: Understand the basic aspects of fermentation processes, sterilizations, and industrial applications.

CO2: Identify approach of chemical process engineering with basic life sciences in developing processes and products.

CO3: Model and analyze biochemical systems and bioreactors.

CO4: Monitor and control bioprocesses.

# Module 1: (13 hours)

Introduction: Fermentation processes, general requirements of fermentation processes – An overview of aerobic and anaerobic fermentation processes and their application in industry - Medium requirements for fermentation processes - examples of simple and complex media, design and usage of commercial media for industrial fermentation. Sterilization: Thermal death kinetics of microorganisms - Batch and Continuous Heat-Sterilization of liquid Media - Filter Sterilization of Liquid Media and Air. Enzyme technology, Enzymes: Classification and properties -Applied enzyme catalysis - Kinetics of enzyme catalytic reactions.

# Module 2: (11 hours)

Microbial metabolism - Metabolic pathways - Protein synthesis in cells. Stoichiometry and Kinetics of substrate utilization, biomass formation, and product formation: Stoichiometry of microbial growth, Substrate utilization and product formation-Batch and Continuous culture, Fed-batch culture Recovery and purification of products. Bioreactor and product recovery operations: Operating considerations for bioreactors for suspension and immobilized cultures, Selection, scale-up, operation of bioreactors.

# Module 3: (15 hours)

Mass transfer in heterogeneous biochemical reaction systems, oxygen transfer in submerged fermentation processes, oxygen uptake rates and determination of oxygen transfer rates and coefficients; the role of aeration and agitation in oxygen transfer. Heat transfer processes in biological systems. Introduction to Instrumentation and Process Control in Bioprocesses: Measurement of physical and chemical parameters in bioreactors - Monitoring and control of dissolved oxygen, pH, impeller speed and temperature in a stirred tank fermenter.

- 1.M.L. Shuler and F. Kargi, Bioprocess Engineering, Basic Concepts, 2nded. New Delhi, India: Prentice Hall of India, 2002.
- 2.J.E. Bailey and D.F. Ollis, Biochemical Engineering Fundamentals, 2nd ed. New York: McGraw-Hill Publishing Co., 2010.
- 3.P. Stanbury, A. Whitakar and S.J. Hall, Principles of Fermentation Technology, 3rd ed. Oxford, UK: Butterworth-Heinemann, 2016.

#### **CH6023D FLUIDIZATION ENGINEERING**

Pre-requisites: Nil Total hours: 39

L	T	Р	С
3	0	0	3

#### **Course Outcomes:**

CO1: Understanding of fluidization behaviour and various fluidization regimes.

CO2: Estimate different empirical correlations for pressure drop, hold up, and different flow models

CO3: Write heat and mass transfer rates and model equations for fluidized beds

CO4: Design a fluidized bed system for different applications.

# Module 1: (12 hours)

Introduction - fluidized state, nature of hydrodynamic suspension, particle forces, species of fluidization, regimization of the fluidized state, operating models for fluidizations systems and application of fluidization systems. Hydrodynamics of fluidization systems - general bed behavior pressure drop, flow regimes, incipient fluidization, pressure fluctuations, phase holdups and measurement techniques.

#### Module 2: (12 hours)

Empirical correlations for solids holdup, liquid holdup and gas holdup, flow models - generalized wake model, structural wake model and other important models. Solids mixing and segregation - phase juxtaposition operation shifts, reversal points, degree of segregation, mixing - segregation equilibrium, generalized fluidization of polydisperse systems, liquid phase mixing and gas phase mixing.

#### Module 3: (15 hours)

Mass transfer – gas-liquid mass transfer, liquid-solid mass transfer, and wall to bed mass transfer. Heat transfer - column wall to bed heat transfer, immersed vertical cylinder to bed heat transfer and immersed horizontal cylinder to bed heat transfer. Miscellaneous systems - conical fluidized bed, moving bed, slurry bubble columns, turbulent bed contactor, two and three phase inverse fluidized bed, draft tube systems, semi-fluidized bed systems, annular systems and typical applications, Geldart's classification for power assessment, powder characterization and modeling by bed collapsing.

- 1. L.S. Fan, Gas-Liquid-Solid Fluidization Engineering, Butterworths, 1989.
- 2. D. Kunni and O. Levenspiel, Fluidization Engineering, Butterworth-Heinemann, 2nd Edition, London, 1991.
- 3. M. Kwauk, Fluidization Idealized and Bubbleless with applications, Science Press, 1992.
- 4. J.F. Davidson and D. Harrison, Fluidization, Academic Press, 1971.
- 5. F.A. Zenz and D.F. Othmer, Fluidization and Fluid Particles Systems, Reinhold Publishing, 1960.

# **CH6024D ENVIRONMENTAL ENGINEERING**

Pre-requisite: Nil Total hours: 39 Course Outcomes:

L	Т	Р	С
3	0	0	3

- CO1: Understand the current environmental problems.
- CO2: Identify clean technology for effluent treatment.
- CO3: Plan strategies to control, reduce and monitor pollution
- CO4: Select the most appropriate technique to purify and control of pollutants.
- CO5: Conversant with basic environmental legislation

# Module 1 (13 hours)

Environmental awareness: Environment-friendly chemical process, hazard and risk analysis, Environmental audits. Clean technology: towards the eco-friendly product of chemical industry, pesticides –their transfer and transportation in the environment, biological and electrical technology for effluent treatments.

#### Module 2 (13 hours)

Chemical Engineering Processes: Unit operations –application of –abatement of water pollution, current strategies to control air pollution, disposal of solid wastes. Recycling methodology: Economic recovery and recycling and reuse of wastes, transport fuel –Biodiesel for a cleaner environment, Biotransformation of toxic chemicals

#### Module 3 (13 hours)

Pollution Prevention: Mass exchange network synthesis for pollution control and minimization implication of environmental constraints for process design, policies for regulation of environmental impacts, the concept of common effluent treatment, environmental legislation, the role of Government and industries.

- 1. Rao, C.S., Environmental pollution control engineering, Wiley Eastern Ltd., 2007.
- 2. Peavy H.S. Rowe D.R. and George Tehobanoglous, Environmental Engineering, McGraw Hill Book Company, NY, 1985.
- 3. Rao M.N. and Rao H.V.N., Air Pollution, Tata McGraw Hill publishing Co.Ltd., 1989.
- 4. Theodore L and Buonicore A.J., Air Pollution Control Equipments. Prentice Hall Inc, NY, 1988.
- 5. Coulson J.M., Richardson J.F. and Sinnott R.K., Chemical Engineering Vol.6, Pergamon Press, 1999.
- 6. Gilbert M.Mastrs, Introduction to Environmental Engineering and Science, Prentice Hall of India, New Delhi, 1998.
- 7. Wahi S.K., Agnihotri A.K., and Sharma J.S., Environmental Management in Petroleum Industry, Wiley Eastern Limited, New Delhi, 1996.
- 8. Smith R., Chemical Process Design, McGraw Hill, NY, 1995.

# **CH6025D BIOLOGICAL WASTEWATER TREATMENT**

L T P C 3 0 0 3

Pre-requisite: Nil Total hours: 39

#### Course outcomes:

CO1: Recognise biochemical operations

CO2: Explain the theory and model the theoretical performance of suspended growth reactors and attached growth reactors

CO3: Apply the knowledge of anaerobic and aerobic biological wastewater treatment processes and engineering on the design of wastewater treatment systems and configurations for the removal of organic matter

CO4: Illustrate the fate and effects of xenobiotic organic chemicals

# Module 1 (15 hours)

Classification of biochemical operations, fundamental of biochemical operations, stoichiometry and kinetics of biochemical operations, theory and modeling of ideal suspended growth reactors, modeling of suspended growth systems, aerobic growth of heterotrophs in a single continuous stirred tank reactor, receiving soluble substrate, multiple microbial activities in a single continuous stirred tank reactor, multiple microbial activities in complex systems, Techniques for evaluating kinetics and stoichiometry parameters.

#### Module 2 (11 hours)

Theory and Modeling of ideal attached growth reactors, biofilm modeling, the aerobic growth of biomass in packed towers, the aerobic growth of heterotrophs in rotating disc reactors, fluidized bed biological reactors.

# Module 3 (13 hours)

Applications of suspended growth reactors, design and evaluation of suspended growth processes, activated sludge, biological nutrient removal, aerobic digestion, anaerobic processes, lagoons, applications of attached growth reactors, trickling filter, rotating biological contactor, submerged attached growth bioreactors, future challenges, fate and effects of xenobiotic organic chemicals.

- 1. Grady, C.P.L, Daigger, G, and Lim, H, C, Biological Waste Water Treatment, 2<sup>nd</sup> Edition, Marcel Dekker, 1999.
- 2. Mizrahi A, Biological Waste Treatment, John Wiley Sons Inc., 1989.

# **CH6026D BIOREACTOR ENGINEERING**

L	T	Р	С
3	0	0	3

Total hours: 39 Pre-requisites: Nil

# **Course Objectives:**

- CO1: Design and analyze batch, continuous flow, and fed batch reactors.
- CO2: Determine the yield coefficients of biomass and product formation
- CO3: Apply the reactor optimization principles for the design of bioreactors for industrially important biological products, primary and secondary products.
- CO4: Determine the mass transfer coefficients and heat transfer coefficients for a biological system.

#### Module 1 (13 hours)

Overview of fermentation processes, media design and sterilization for fermentation processes, general requirements of fermentation industry, basic design and construction of a fermentor and its ancillaries, materials of construction, vessel geometry, flow measuring devices, valves (basic construction features), medium requirements for fermentation processes, examples of simple and complex media, design and usage of commercial media for industrial fermentations, thermal death kinetics of microorganisms, batch and continuous heat-sterilization of liquid media, filter sterilization of liquid media and air sterilization, radiation and chemical sterilization, sterilization equipment – batch and continuous.

#### Module 2 (12 hours)

Metabolic stoichiometry and bioenergetics, thermodynamics, mass and energy balances in microbial metabolism, cell growth and product formation, metabolic heat generation, stoichiometry of cell growth and product formation - elemental balances, available - electron balances, degrees of reduction of substrate and biomass, yield coefficients of biomass and product formation, maintenance coefficients, oxygen consumption and heat evolution in aerobic cultures.

# Module 3 (14 hours)

Transport phenomena in bioreactors, mass transfer in the heterogeneous biochemical reaction system, oxygen transfer in submerged fermentation processes, oxygen uptake rates and determination of oxygen transfer coefficients, the role of aeration and agitation in oxygen transfer, heat transfer processes in the biological system. Process design and operation of bioreactors, operational modes of reactors – batch, continuous, fed-batch, repetitive batch, recycle and continuous cultivation, novel bioreactors, stirred tank, airlift and loop reactor, packed – bed and hollow – fibre membrane bioreactors, reactors for waste – treatment processes, scale-up criteria for bioreactors.

- 1. Bailey, J.E. and Ollis, D.F., Biochemical Engineering Fundamentals, McGraw Hill, 28<sup>th</sup> Jan 2010.
- 2. Shule and Kargi, Bioprocess engineering, Prentice Hall, Second Indian Reprint, 2004.
- 3. Karl Schugerl, Bioreaction Engineering (Volume 3), John Wiley, 1997.
- 4. T.K. Ghose (Ed.), Process Computations in Biotechnology, Tata McGraw Hill, 1994.
- 5. Atkinson, B. and Mavituna, F., Biochemical Engineering and Biotechnology Handbook, 6, McGraw Hill, 2<sup>nd</sup> Edition, 1993.
- 6. H.J. Rehm and G. Reed (Ed.), Biotechnology (Vol. 3, Bioprocessing), VCH, 1993.
- 7. Harvey W. Blanch and Duoglas S. Clark, Biochemical Engineering, Marcel Dekker Inc., 1997.
- 8. Pauline Doran, Bioprocess Engineering Principles, Academic Press, 2012.

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# **CH6027D SAFETY MANAGEMENT IN PROCESS INDUSTRIES**

Pre-requisites: Nil Total hours: 39 Course Outcomes:

L	Т	Р	С
3	0	0	3

- CO1: Knowledge of the safety aspects of design, erection, and commissioning of chemical plants.
- CO2: Analyze safety and hazards in operations, maintenance, storage and handling of chemicals.
- CO3: Examine toxic release, control methodologies and safety consideration specific to common chemicals.
- CO4: Carry out various risk assessment techniques.

# Module 1: (13 hours)

Safety in the design process of chemical plants, safety in erection and commissioning of chemical plants, safety in material handling, pressure and leak testing. Safety in operations and maintenance, exposure of personnel, operational activities and hazards, work permit systems, entry into confined space with toxic contaminants.

#### Module 2: (15 hours)

Safety in storage and handling of chemicals and gases, hazards during transportation, pipeline transport, safety in chemical laboratories. Toxic release and control methodologies, toxic effects, threshold limit values, awareness and preparedness for energy at local level. Specific safety consideration for cement, paper, pharmaceutical, petroleum, petrochemical, rubber, fertilizer, and distilleries.

#### Module 3: (11 hours)

Risk assessment - hazard vs risk, techniques for risk assessment, qualitative, rapid and comprehensive risk assessment techniques: checklists, indices, HAZOP, maximum credible accident analysis, fault tree analysis, past accident analysis, FMEA, quantitative risk assessment, domino effect and its assessment.

- 1.Lees, F.P., Loss Prevention in Process Industries, Butterworths, NewDelhi, 4thEdn., Aug 2012.
- 2. Accident Prevention Manual for Industrial Operations, NSC, Chicago, 1982.
- 3.Khan, F.I., and Abbasi, S.A., Risk Assessment in Process Industries: Advanced Techniques, DiscoveryPublishing House, New Delhi, 1st Edn., 2004.
- 4. Abbasi, T, and Abbasi, S.A., Boiling Liquid Expanding Vapour Explosions, Springer-verlag, 1st Edn., 2007.

# CH6028D FIRE ENGINEERING AND EXPLOSION CONTROL

Pre-requisites: Nil Total hours: 39 Course Outcomes:

L	Т	Р	С
3	0	0	3

CO1: Understand the physical and chemical properties and dynamics of fire and combustion.

CO2: Understand fire and explosion protection systems.

CO3: Analyse fire and safety measures.

CO4: Develop firefighting skills.

# Module 1: (15 hours)

Fire chemistry, dynamics of fire behavior, fire properties of solid, liquid and gas, fire spread, the toxicity of products of combustion. Industrial fire protection systems – sprinkler, hydrants, standpipe. Special fire suppression system like deluge and emulsifier.

# Module 2: (15 hours)

Explosion protection systems, explosion parameters, explosion suppression systems, hazards in L.P.G handling. Building evaluation for fire safety, fire load, fire resistant materials and fire testing, structural fire protection, exits, and egress.

# Module 3: (9 hours)

Statutory rules and techniques of firefighting, Indian explosive acts, and rules, techniques of firefighting and demonstration.

- 1. James, D., Fire Prevention Handbook, Butterworths, London, 1986.
- 2. Gupta R.S., Handbook of Fire Technology, Orient Longman, Bombay, 2005.

# **CH6029D FIRE MODELING AND DYNAMICS**

Pre-requisites: Nil Total hours: 39 Course Outcomes:

Ш	Τ	Р	O
3	0	0	3

CO1: Knowledge of the flammability and explosive characteristics of hydrocarbons and petrochemicals

CO2: Knowledge of diffusion flames and fire plumes

CO3: Model fires and explosions

CO4: Monitor and control spread of fire and smoke

# Module 1: (9 hours)

Introduction, properties of hydrocarbons and petrochemicals, flammability characteristics, explosive characteristics, fuels and the combustion process, the nature of fuels, thermal decomposition and stability of polymers, the ideal gas law, vapor pressure of liquids, combustion and energy release, the mechanism of gas-phase combustion, temperatures of flames, limits of flammability, measurement of flammability limits, characterization of the lower flammability limit, dependence of flammability limits on temperature and pressure, flammability diagrams.

# Module 2: (15 hours)

The structure of a premixed flame, heat losses from premixed flames, measurement of burning velocities, a variation of burning velocity with experimental parameters. Diffusion flames and fire plumes, laminar jet flames, turbulent jet flames, flames from natural fires, buoyant plume, fire plume, interaction of fire plume with compartment boundaries, effect of wind on the fire plume, radiation from flames, response of ceiling-mounted fire detectors, interaction between sprinkler sprays and fire plume, removal of smoke. Modeling fires - pool fires, torch/flares, fireballs, jet fires, vapor cloud fires. Modeling releases - release rate, aerosol formation, pool vaporization. Modeling vapor cloud dispersion - cloud formation, source models, aerosols, pool vaporization, dense gas dispersion, momentum jet dispersion.

# Module 3: (15 hours)

Explosions - TNT Models, TNO Multi-Energy, Baker-Strehlow model; modeling vapor cloud explosions, confined spaces, open-air explosions, BLEVE's, computer simulation of fires in buildings, engineering forensic tools and use of computer fire models in fire investigation and protection. Spread of flame over liquids and solids, environmental effects, flame spread modeling, spread of flame through open fuel beds, applications, radiation-enhanced flame spread, rate of vertical spread; the production and movement of smoke- production and measurement of smoke, production of smoke particles, measurement of particulate smoke, methods of test for smoke production potential, forces responsible for smoke movement, rate of smoke production in fires, smoke control in large spaces, smoke control in shopping centers, smoke control on protected escape routes.

- 1. Drysdale D., An Introduction to Fire Dynamics, 3rd Edn., John Wiley & Sons, 2011.
- 2. CCPS, Guidelines for Fire Protection in Chemical, Petrochemical, and Hydrocarbon Processing Facilities, Center for Chemical Process Safety, 2003.
- 3. Abbasi, T., Abbasi, S.A., The Boiling Liquid Expanding Vapour Explosion (BLEVE): Mechanism, Consequence Assessment, Management, 2007.
- 4. Dr. Mannan, S., Lee's Loss Prevention in the Process Industries Hazard Identification, Assessment and Control,4th Edn., Vols.1–4, Elsevier, Butterworth-Heinemann, Oxford, 2012.
- 5. CCPS, Guidelines for Chemical Process Quantitative Risk Analysis, 2nd Edn., Center for Chemical Process Safety, American Institute of Chemical Engineers, New York, 2000.

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#### CH6030D ADVANCED POLYMER TECHNOLOGY

Prerequisite: Nil Total hours: 39

L	Т	Р	С
0	3	0	3

#### Course outcomes:

CO1: Classify polymers based on conformation and configuration

CO2: Describe the mechanism of polymerization and methods of polymerization

CO3: Explain the glass transition temperature and crystalline behaviour of the polymers

CO4: Elucidate the role of polymer additives in polymer behaviour

CO5: Explain the influence of process variable on the properties of polymers

#### Module 1 (13 hours)

General introduction to polymers with emphasis on important concepts such as monomer, functionality and physical state (amorphous and crystalline), classification of polymers on the basis of source, elemental composition, heat, chemical reactivity, chemical/monomer composition, geometry, and stereoregularity. Chain Configurations: conformation of polymers-constitutional isomerism, positional isomerism, branching; Configurational isomerism-geometrical isomerism, stereo isomerism; polymer conformation-conformation of small molecules and conformation of polymers; conformation of macromolecules-general shape of macromolecules –general shape of macromolecules; Chemistry and mechanism of polymerization: definition of polymerization, factors affecting polymerization, chain (addition) polymerization (free radical, ionic and co-ordination polymerizations), step (condensation) polymerization-molecular weight in step growth polymerization, kinetics of step growth polymerization; polyaddition polymerization, ring opening polymerization, copolymerization – introduction, free radical, ionic and copoly-condensation (with examples).

# Module 2 (13 hours)

Methods of polymerization: Bulk, solution, precipitation polymerization, suspension, emulsion, melt polycondensation, interfacial polymerization, solution polycondensation, solid phase, gas phase and (formulation, mechanism, properties of the polymer produced, advantages and disadvantages of each technique). Structure of Crystalline Polymers: Early studies: The fringed-micelle model, polymer single crystal: Folded chain model, the switchboard model. Crystallization from melt: Sperulitic morphology, mechanism of spherulite formation, spherulite of polymer blends and blocks. Kinetics of crystallization: experimental observations of crystallization kinetics, theories of crystallization kinetics: Avrami equation. Glass transition temperature: definition, glassy region and glass transition region, rubbery plateau region, rubbery flow region, liquid flow region, states of aggregation, Factors influence the glass transition temperature, Tg and Molecular weight, Tg and plasticizers, Tg and copolymers, Tg and Tm, Importance of Tg.

# Module 3 (13 hours)

Influence of the process variables on the Properties- introduction, orientation,- degree of orientation, measurement of degree of orientation, uniaxial orientation – its meaning, change of properties by orientation in amorphous and crystalline polymers; biaxial orientation; quantitative relationships for some physical quantities after orientation like density, thermal expansion, thermal conductivity, refractive index (birefringence), modulus of elasticity, mechanical damping, generalized stress-strain relationship for polymers. Effect of additives on polymers in their behaviour- fillers, reinforcements, coupling agents, antioxidants, UV stabilizers, flame retardants, plasticizers, lubricants, heat stabilizers, impact modifiers, other additives.

- 1. Fred W. Billmeyer, Jr., Textbook of Polymer Science, John Wiley & Sons, New York. 2008.
- 2. P.J. Flory, Principles of Polymer Chemistry, Cornell University Press, Ithaca, NY 2007.
- 3. V.R. Gowariker, N.V.Viswanathan, J. Sreedhar, Polymer Science, New Age International (P) Ltd., New Delhi, 2003.
- 4. Joel R Fried, Polymer Science, and Technology, Prentice-Hall of India Pvt. Ltd., New Delhi, 2012.
- 5. N.G. McCrum, C.P. Buckley and C.B. Bucknall, Principles of Polymer Engineering, Oxford Science publications, 1997.
- 6. R.J. Crawford, Plastics Engineering, Butterworth-Heinemann, 2002.
- 7. Raymond B. Seymour and E.C.Charles, Structure -Properties Relationships of Polymers, Plenum Press, New York, 1984.
- 8. Patrick Meares, Polymers-Structure and Bulk Properties, Van Nostrand Pub., New York, 1971.

# **CH6031D MULTIPHASE SYSTEMS AND REACTORS**

Pre-requisite: Nil Total hours: 39

L	Т	Р	C
0	3	0	3

#### **Course Outcomes:**

CO1: Explain the types of multiphase reactors in process industries

CO2: Quantify the hydrodynamic effects in multiphase systems and reactors

CO3: Develop simple mathematical models in multiphase flows

CO4: Develop relations of momentum, energy and material balances in multiphase systems and reactors

# Module 1 (14 hours)

Fundamental concepts of multiphase: gas -liquid, gas-solid, liquid-liquid and liquid-solid systems. Particle drop and bubble dynamics, Application of continuity, momentum and energy equations. Hydrodynamic characteristics: hold up, slip, pressure drop and rise/drop velocities.

#### Module 2 (13 hours)

Mass and energy transfer with and without simultaneous chemical reactions, application to trickle beds, bubble and slurry reactors, cyclones, fluidized beds etc. Gas-liquid-solid catalytic and non-catalytic reacting systems, Interaction of physical and chemical inter and intra-particle transport.

# Module 3 (12 hours)

Development of kinetic models, isothermal and nonisothermal systems, stability criteria. Flow Modeling. Hydrodynamic, deterministic and stochastic description, Evaluation of model parameters, Interfacial area, Bubble/drop breakup, distributions, coalescence, and dynamics.

- 1. G.F., Froment K.B. Bischoff, Chemical Reactor Analysis and Design, 3rd ed., John Wiley, New York, 2010.
- 2. G.W Wallis, One Dimensional Two-Phase Flow, McGraw-Hill, New York, 1989.
- 3. Gianetto A. and Selveston P.L., Multiphase Chemical Reactors, Hemisphere Publishing Corporation, New York., 2006.

# **CH6032D ADVANCED TRANSPORT PHENOMENA**

Pre-requisite: Nil Total hours: 39

L	Т	Р	C
3	0	0	3

#### **Course Outcomes:**

- CO1: Demonstrate the physics behind the transport of momentum, heat and mass transport
- CO2: Derive the fundamental transport equations that govern momentum, heat and mass transfer and associated initial and boundary conditions
- CO3: Demonstrate the mechanisms for momentum transfer its influence on heat and mass transfer
- CO4: Develop models and suitable assumptions for their simplification without the loss of generality
- CO5: Apply mathematics and numerical methods to solve the governing equations both analytically and numerically

# Module 1 (14 hours)

Equations of change for isothermal systems, Velocity distributions with more than one independent variable, Velocity distributions in turbulent flow, Interphase transport in isothermal systems, Macroscopic balances for isothermal systems.

# Module 2 (12 hours)

Temperature distributions in solids and in laminar flow, Equations of change for non-isothermal systems, Temperature distributions with more than one independent variable, Temperature distributions in turbulent flow, Interphase transport in nonisothermal systems. Macroscopic balances for nonisothermal systems.

# Module 3 (13 hours)

Concentration distributions in solids and in laminar flow, Concentration distributions with more than one independent variable, Concentration distributions in turbulent flow. Interphase transport in multi-component systems, Macroscopic balances for multi-component systems.

- Bird R.B., Stewart W.E., and Light Foot E.N., Transport Phenomena 2<sup>nd</sup> Ed., Wiley International Edition, 2007.
- 2. Christie J. Geankopolis, Transport processes, and unit operation, 3<sup>rd</sup> Ed., Prentice Hall (India) Pvt., Ltd., New Delhi, 1997.
- 3. C.O. Bennett and J.E.Myers, Momentum, heat and mass transfer, 3<sup>rd</sup> Ed., McGraw Hill, 1982.

# CH6033D NUMERICAL METHODS IN CHEMICAL ENGINEERING

Pre-requisite: Nil Total hours: 39

L	Т	Р	С
0	3	0	3

#### **Course Outcomes:**

- CO1: Formulate chemical engineering problems as mathematical models and apply appropriate solution strategies for accurate solutions
- CO2: Analyze the chosen numerical strategy and find an alternate strategy when it is required
- CO3: Choose and adopt appropriate computational requirements of the various solution options and apply the knowledge for the successful solution of the given problem
- CO4. Select appropriate software tool or package for the solution to a chemical engineering problem.
- CO5: Solve process design problems using the numerical techniques for the mathematical models of chemical processes

# Module 1 (11 hours)

Design and analysis of experiments: Treatment and interpretation of engineering data: Curve fitting, Non-linear least square regression. Interpolation: Newton's Forward/Backward interpolation formula, Lagrange's interpolation formula and experiments their application. Tests of significance, Analysis of variance.

# Module 2 (13 hours)

Formulation of physical problems: Mathematical statement of the problem, Representation of problems, Formulation on Socuene extraction in single & multiple stages, Radial heat transfer through a cylindrical conductor, salt accumulation in a stirred tank. Numerical solution of linear & nonlinear algebraic equations: Linear systems of equations, solutions by Creamer's Rule, Matrix methods, Gaussian, Gauss-Jordan, Jacobean, Gauss-Seidel and Relation methods. Non-linear equations: Bisection, Regula-falsi, Secant and Newton- Raphson methods.

#### Module 3 (15 hours)

Numerical solution of ordinary differential equations: Ordinary differential equations: Runge- Kutta, Euler's and Milne's predictor-corrector methods. A solution of boundary value problems. Finite differences: Finite differences, Partial differential equations, Solutions of elliptic, parabolic, and hyperbolic types of equations.

- 1. S. K. Gupta, Numerical Techniques for Engineers, Wiley Eastern, 1995.
- 2. M. K. Jain, S.R.K. Iyengar and R. K. Jain, Numerical Methods for Scientific and Engineering Computations, 2004.
- 3. H.S. Mickley, T. K. Sherwood, and C.E. Reed, Applied Mathematics in Chemical Engineering, 2nd Ed., Tata McGraw Hill, New Delhi, 1990.