

# DEPARTMENT OF CHEMICAL ENGINEERING

## SCHEME OF INSTRUCTIONS AND SYLLABUS FOR POST GRADUATE STUDY

M. Tech in Chemical Engineering



**Visvesvaraya National Institute of Technology, Nagpur**

July 2015

# MISSION AND VISION OF VISVESVARAYA NATIONAL INSTITUTE OF TECHNOLOGY, NAGPUR



## MISSION

The Mission of VNIT is to achieve high standards of excellence in generating and propagating knowledge in engineering and allied disciplines. V.N.I.T. is committed to providing an education that combines rigorous academics with joy of discovery. The Institute encourages its community to engage in a dialogue with society to be able to effectively contribute for the betterment of humankind.

## VISION

To contribute effectively to the national endeavour of producing quality human resource of world class standard by developing a sustainable technical education system to meet the changing technological needs of the Country, incorporating relevant social concerns and to build an environment to create and propagate innovative technologies for the economic development of the Nation.

**MISSION AND VISION  
OF  
DEPARTMENT OF CHEMICAL ENGINEERING, V. N. I. T. Nagpur**



**MISSION**

To be a globally recognized chemical engineering program coupled with excellence in education, training, research and consultancy in Chemical Engineering and to serve as a valuable resource for industry and society.

**VISION**

To provide students with updated knowledge in science and technology, to become competent and practicing Chemical Engineers without compromising professional ethics and moral values.  
To undertake research of a caliber that is internationally recognized.  
To undertake collaborative projects which provide opportunities for long-term interaction with academia, industry and other research organizations.  
To develop infra-structure that promotes creativity and an entrepreneurial culture.  
To foster ethical leadership and activities that supports the administration, advancements, governance and regulation of Chemical Engineering education and the engineering profession.

Department of Chemical Engineering offers one M. Tech program, namely, *M. Tech. in Chemical Engineering*. These are four semester program, wherein student has to complete certain number of credits as indicated in Table 1. Each subject (or course) has certain number of credits. There are two types of subjects: Core and elective. Core courses are compulsory and some courses from electives are to be taken to complete the required credits.

**TABLE 1. CREDIT REQUIREMENTS FOR POST GRADUTE STUDIES**

Postgraduate Core (PC)		Postgraduate Elective (PE)	
Category	Credit	Category	Credit
Departmental Core (DC)	36	Departmental Electives (DE)	16
Total	36	Total	16
<b>Grand Total PC + PE</b>			<b>52</b>

The number of credits attached to a subject depends on number of classes in a week. For example a subject with 3-0-0 (L-T-P) means it has 3 Lectures, 0 Tutorial and 0 Practical in a week. This subject will have three credits ( $3 \times 1 + 0 \times 1 + 0 \times 1 = 3$ ). If a student is declared pass in a subject, then he/she gets the credits associated with that subject. Depending on marks scored in a subject, student is given a Grade. Each grade has got certain grade points as follows:

Grades	AA	AB	BB	BC	CC	CD	DD	FF
Grade Points	10	09	08	07	06	05	04	Fail

The performance of a student will be evaluated in terms of two indices, viz. the Semester Grade Point Average (SGPA) which is the Grade Point Average for a semester and Cumulative Grade Point Average (CGPA) which is the Grade Point Average for all the completed semesters at any point in time. SGPA & CGPA are:

$$SGPA = \frac{\sum_{\text{semester}} (\text{Course credits} \times \text{Grade points}) \text{ for all courses except audit}}{\sum_{\text{semester}} (\text{Course credits}) \text{ for all courses except audit}}$$

$$CGPA = \frac{\sum_{\text{All semester}} (\text{Course credits} \times \text{Grade points}) \text{ for all courses with pass grade except audit}}{\sum_{\text{All semester}} (\text{Course credits}) \text{ for all courses except audit}}$$

Students can Audit a few subjects. i.e., they can attend the classes and do home work and give exam also, but they will not get any credit for that subject. Audit subjects are for self enhancement of students.

## **Programme: M. Tech. in Chemical Engineering**

### **Programme Educational Objectives of M. Tech. in Chemical Engineering**

1. To prepare students for successful practice in diverse fields of chemical engineering such as pharmaceuticals, chemicals, polymers / advanced materials, energy, biotechnology and environmental engineering and in the fields of societal expectations on time.
2. To prepare students for advanced studies in Chemical Engineering and its allied fields.
3. To ensure our students are recognized for excellence and leadership and selected for high-ranking industrial, academic, government and other professional positions.
4. To develop students' skills and awareness to become socially, ethically and morally responsible individual in all the challenges they take over in our communities and in the field of chemical engineering.

### **Programme Outcomes of M. Tech. in Chemical Engineering**

- a.
  1. An ability to identify, formulates, and solve engineering problems.
  2. An ability to identify, formulates, and solve engineering problems.
  3. An ability to identify, formulates, and solve engineering problems.
- b. An ability to design a system, component, or process to meet desired needs.
- c. An ability to design and conduct experiments, as well as to analyze and interpret data.
- d. An ability to communicate effectively.
- e.
  1. An understanding of professional and ethical responsibility.
  2. An understanding of professional and ethical responsibility.
- f. An ability to function on multidisciplinary teams.
- g. The broad education necessary to understand the impact of engineering solutions in a global and societal context.
- h. A recognition of the need for, and an ability to engage in lifelong learning.
- i. A knowledge of contemporary issues.

**Overall Credit Structure for M. Tech. Program in Chemical Engineering at VNIT**

**From Academic Year 2015-16**

<b>Category</b>	<b>Credits</b>
Basic Sciences + Engineering Sciences	00
Departmental Core (DC)	36
Departmental Elective (DE)	16
Humanities & Management (HM)	00
Open Course (OC)	00
<b>Total</b>	<b>52</b>

**SCHEME OF INSTRUCTION FOR M. TECH (CHEMICAL ENGINEERING) 2015-16 ONWARD**

Code	Course	L-T-P	Cr	Code	Course	L-T-P	Cr
<b>I Semester</b>				<b>II Semester</b>			
<b>Core</b>				<b>Core</b>			
CML 501	Thermodynamics of Phase and Chemical Equilibria	3-0-0	3	CML 505	Industrial Process Control	3-0-0	3
CML 502	Chemical and Catalytic Reaction Engineering	3-0-0	3	CML 506	Process Analysis, Simulation and Design	3-0-0	3
CML 503	Momentum, Mass, & Heat Transfer	3-0-0	3	CML 507	Novel Separation Processes	3-0-0	3
CML 504	Mathematical Methods in Chemical Engineering	3-0-0	3	CMP 510	Advance Separation Laboratory	0-0-2	1
CMP 508	Analytical and Instrumental Laboratory	0-0-2	1				
CMP 509	Computational and Design Laboratory	0-0-2	1				
<b>Elective (Any Two)</b>				<b>Elective (Any Two Theory + Any One Practical)</b>			
CML 521	Chemical Engg. Computational Fluid Dynamics	3-0-0	3	CML 522	Membrane Separation Processes	3-0-0	3
CML 528	Interfacial Science and Engineering	3-0-0	3	CML 523	Petroleum Engineering	3-0-0	3
CML 529	Optimization Techniques in Process Design	3-0-0	3	CML 524	Polymer Science and Engineering	3-0-0	3
CML 536	Analysis and Design of Experiments*	3-0-0	3	CML 535	Advanced Nanotechnology	3-0-0	3
CML 533	Mass Transfer with Chemical Reaction	3-0-0	3	CML 525	Catalysis: Theory and Practice	3-0-0	3
CML 527	Mineral Beneficiation			CML 534	Reliability Analysis in Process Industry	3-0-0	3
				CMP 541	Advance Chemical Process Laboratory	0-0-2	1
				CMP 542	Advance Process Simulation Laboratory	0-0-2	1
<b>Total</b>			<b>20</b>	<b>Total</b>			<b>17</b>
<b>III Semester</b>				<b>IV Semester</b>			
<b>Core</b>				<b>Core</b>			
CMD 509	Project Phase I	0-0-6	3	CMD 510	Project Phase II	0-0-18	9
<b>Elective (Any One)</b>							
CML 530	Process Intensification	3-0-0	3				
CML 532	Energy Technology and Conservation	3-0-0	3				
CML 526	Total Quality Management	3-0-0	3				
<b>Total</b>			<b>6</b>	<b>Total</b>			<b>9</b>

**List of Core Subjects:**

<b>Course Code</b>	<b>Course Title</b>	<b>L-T-P-C</b>
CML 501	Thermodynamics of Phase and Chemical Equilibria	3-0-0-3
CML 502	Chemical and Catalytic Reaction Engineering	3-0-0-3
CML 503	Momentum, Mass, & Heat Transfer	3-0-0-3
CML 504	Mathematical Methods in Chemical Engineering	3-0-0-3
CML 505	Industrial Process Control	3-0-0-3
CML 506	Process Analysis, Simulation and Design	3-0-0-3
CML 507	Novel Separation Processes	3-0-0-3
CMP 508	Analytical and Instrumental Laboratory	0-0-2-1
CMP 509	Computational and Design Laboratory	0-0-2-1
CMP 510	Advance Separation Laboratory	0-0-2-1
CMD 511	Project Phase I	0-0-6-3
CMD 512	Project Phase II	0-0-18-9
	<b>Total Credit : 36</b>	

**List of Elective Subjects (Total credits to be taken = 16)**

CML 521	Chemical Engg. Computational Fluid Dynamics	3-0-0-3
CML 522	Membrane Separation Processes	3-0-0-3
CML 523	Petroleum Engineering	3-0-0-3
CML 524	Polymer Science and Engineering	3-0-0-3
CML 525	Catalysis: Theory and Practice	3-0-0-3
CML 526	Total Quality Management	3-0-0-3
CML 527	Mineral Beneficiation	3-0-0-3
CML 528	Interfacial Science and Engineering	3-0-0-3
CML 529	Optimization Techniques in Process Design	3-0-0-3
CML 530	Process Intensification	3-0-0-3
CML 531	Environmental Management Systems	3-0-0-3
CML 532	Energy Technology and Conservation	3-0-0-3
CML 533	Mass Transfer with Chemical Reaction	3-0-0-3
CML 534	Reliability Analysis in Process Industry	3-0-0-3
CML 535	Advanced Nanotechnology	3-0-0-3
CML 536	Analysis and Design of Experiments	3-0-0-3
CMP 541	Advance Chemical Process Laboratory	0-0-2-1
CMP 542	Advance Process Simulation Laboratory	0-0-2-1



# **SYLLABUS**

**List of Core Subjects:**

<b>Course Code</b>	<b>Course Title</b>	<b>L T P C</b>
CML 501	Thermodynamics of Phase and Chemical Equilibria	3 0 0 3
CML 502	Chemical and Catalytic Reaction Engineering	3 0 0 3
CML 503	Momentum, Mass, & Heat Transfer	3 0 0 3
CML 504	Mathematical Methods in Chemical Engineering	3 0 0 3
CML 505	Industrial Process Control	3 0 0 3
CML 506	Process Analysis, Simulation and Design	3 0 0 3
CML 507	Novel Separation Processes	3 0 0 3
CMP 508	Analytical and Instrumental Laboratory	0 0 2 1
CMP 509	Computational and Design Laboratory	0 0 2 1
CMP 510	Advance Separation Laboratory	0 0 2 1
CMD 509	Project Phase I	0 0 6 3
CMD 510	Project Phase II	0 0 18 9
	<b>Total Credit : 36</b>	

**CML 501: Thermodynamics of Phase and Chemical Equilibria**

[(3-0-0); credits:3]

**Objective:** To train students on thermodynamics and equilibria, physical interpretation, molecular dynamics and cooperative phenomenon

**Syllabus:** Elementary Statistical Mechanics, Postulates, Ensembles, Relation between microscopic and macroscopic thermodynamics; Equivalence of ensembles, Legendre Transformation. Intermolecular Potential Energy functions (Non-Polar molecules); Distribution functions: Radial Distribution Function (RDF)

Physical Interpretation: Structure of Fluids and Solids, Experimental Measurement Thermodynamics from RDF; Molecular Simulation Techniques: Mass, Length and Time Scales at atomic levels, LJ reduced units, Molecular Dynamics: Autocorrelation Functions: Transport properties; Random Walks; Diffusion and Einstein's Equation; Stochastic: Monte Carlo Numerical Integration versus Monte Carlo Integration Importance Sampling, Markov Chains, Metropolis Monte Carlo Metropolis MC applied to NVE ensemble (eg. Demon Algorithm), NVT ensemble, NPT ensemble and VT ensemble Applications of Statistical Mechanics: Thermo- physical property calculations in ensembles;

Cooperative Phenomenon: Phase Equilibria: Ising model, Gibbs Ensemble (VLE), Thermodynamic Integration, Gibbs-Duhem Integration, Free Energy Evaluation; Virial EOS: second virial coefficient;

Special Applications: Einstein Crystal; Self Assembly; Polymer Solution

**References:**

1. Borgnakke and Sonntag, Fundamentals of Thermodynamics, Wiley, 2008.
2. Vincenti and Kruger, Introduction to Physical Gas Dynamics, Wiley 1966.
3. Hansen, J.B., and McDonald, I.R., Theory of Simple Liquids, Academic, 1990.
4. McQuarrie, D.A., Statistical Mechanics, Viva Books, 2003.
5. Tester, J.W., and Modell, M., Thermodynamics and its Applications, Third Edn, Prentice Hall, 1997.
6. Callen, H.B., Thermodynamics and an Introduction to Thermostatistics, John Wiley & Sons, 1985.
7. McQuarrie, D.A., Statistical Mechanics, University Science Books, 2000.
8. Hill, T.L., An Introduction to Statistical Thermodynamics, Dover

**CML 502: Chemical and Catalytic Reaction Engineering**

[(3-0-0); credits:3]

**Objective:** To train students on multiphase reactor engineering, its importance, kinetics, design aspects and process intensification.

**Syllabus:** Review on Chemical Reaction Engineering

Introduction to Multiphase Reactor Engineering

Types, classification, application of industrial importance reactors

Hydrodynamic characteristics of different reactors

Kinetics and Design aspects of multiphase reactors

Process Intensification and Special Reactors

Introduction to CFD for reactor design

**References:**

1. Heterogeneous reactions: Analysis, examples, and reactor design. L. K. Doraiswamy and M. M. Sharma, John Wiley and Sons, New York, 1984, Vol. I and II.
2. Fluid Mixing and Gas Dispersion in Stirred Reactors, G.B. Tatterson, McGraw Hill Inc. New York, 1991
3. Fluid Mixing and Gas Dispersion in Stirred Reactors, G.B. Tatterson, McGraw Hill Inc. New York, 1991
4. Bubble-column Reactors, W.D. Deckwer, J. Wiley, New York [modeling, scale-up and design], 1989
5. Fluidization Engineering, D. Kunii and O. Levenspiel, Butterworth-Heinemann, Boston – [design and modeling of fluidized-bed reactors], 1991. Chemical Reactor Analysis, G. F. Froment and K. B. Bischoff, John Wiley & Sons, Singapore, 1990 2<sup>nd</sup> Edition.
6. Chemical Reaction Engineering, Octave Levenspiel, John Wiley & Sons, Singapore, 1998 3<sup>rd</sup> Edition.
7. Elements of Chemical Reaction Engineering, Fogler H.S., Prentice-Hall, NJ, 2006, 4<sup>th</sup> Edition
8. Chemical Engineering Kinetics, Smith J. M., McGraw Hill, N Y, 1981, 3<sup>rd</sup> Edition.

**CML 503: Momentum, Mass, & Heat Transfer****[(3-0-0); credits:3]****Objective:** To train students on advances in momentum, mass and heat transfer.**Syllabus:** Viscosity and Mechanisms of Momentum Transport, Shell momentum balances and velocity distribution in Laminar flow., Equation of continuity, Mechanical energy, and equation of motion, velocity distribution in Turbulent flow, Polymeric liquids, Non Newtonian Viscosity and Models, Molecular theory of Polymeric Liquids. Boundary layer flow and hydrodynamic boundary layer. Thermal conductivity and the mechanism of Energy transport, Shell energy balance and temperature distributions in laminar and turbulent flow, convective transport of energy, Thermal boundary layer theory, Heat transfer coefficients for different situations. Diffusivity and the mechanisms of Mass Transport. Mass transport by convection, concentration distributions in laminar and turbulent flow. concentration boundary layer, Mass transfer with chemical reaction. Simultaneous heat, mass and momentum transfer, analogy, dimensional analysis, Scale up. Recent Developments in the fields and future challenges.**References:**

1. Transport Phenomena, R.B.Bird, W.E. Stewart and E.W. Lightfoot. John Wiley, 2nd Ed
2. Fundamentals of Momentum, Heat and Mass Transfer, J.R. Wilty, et. Al. John Wiley, 4th Ed.
3. Transport Processes and Separation process Principles, Christie J. Geankopolis 4th Ed. Prantice Hall

**CML 504: Mathematical Methods in Chemical Engineering****[(3-0-0); credits:3]****Objective:** To train students on advances in mathematical techniques and numerical methods and its application in chemical engineering.**Syllabus:** An introduction to mathematical modelling and simulation; vector and tensor spaces; metric, norm and inner products; orthonormalization; matrices, operators and transformations; eigen values and eigen vectors; Fredholm alternative, Rayleigh quotient and its application to chemical engineering systems; self adjoint and non-self adjoint systems; partial differential equations and their applications in chemical engineering; Sturm-Louisville theory; separation of variables and Fourier transformations; application of Greens function for solution of ODE and PDEs in chemical engineering; numerical techniques for solution of ODE and PDEs such as Runge Kutta Techniques; Predictor corrector methods; implicit and explicit techniques for PDEs; finite difference method for PDEs; linear stability and limit cycles; bifurcation theory; secondary bifurcation and chaos; Role of computer programming like 'C' and packages like MATLAB in problem solving; Linear algebraic equations; Solution of non-linear algebraic equations; Newton Raphson technique and homotopy.**References:**

1. Santosh K. Gupta, Numerical Methods for Engineers, 2<sup>nd</sup> Edition, New Age International (P) Ltd., New Delhi.
2. Steven C. Chapra & Raymond P Canale, Numerical Methods for Engineers, 4th Edition, Tata McGraw Hill, New Delhi.
3. Bruce A. Finlayson, Lorenz T. Biegler, Ignacio E. Grossmann, Mathematics in Chemical Engineering, 2006 Wiley-VCH Verlag GmbH & Co.
4. Gilbert Strang, Linear Algebra and its applications, Harcouth Brace Jovanovich, 1988.

**CML 505: Industrial Process Control****[(3-0-0); credits:3]****Objective:** To train students on advances in control system design, process identification, discrete time systems, and model predictive control.**Syllabus:** Review of dynamic behaviour of linear systems and their control system design. Linear processes with difficult dynamics. Nonlinear process dynamics; phase-plane analysis; multiple steady-state and bifurcation behaviour; Process Identification; Controller design via frequency response analysis; Model based control; Cascade, feed-forward & ratio control; Controller design for nonlinear systems; Introduction to multivariable systems. Interaction analysis and multiple single loop design. Design of multivariable controllers; Introduction to sampled data systems; Tools of discrete-time systems analysis; Dynamic analysis of discrete-time systems; Design of digital controllers; Introduction to model predictive control; Convolution models; Model predictive control of MIMO systems.**References:**

1. Stephanopoulos G., "Chemical Process Control", Prentice Hall, 1984.
2. Coughanowr D.R. and LeBlanc S., "Process Systems Analysis and Control", 3rd Ed., McGraw Hill, 2008.
3. Seborg D.E., Edgar T.F. and Mellichamp D.A., "Process Dynamics and Control", 3rd Ed., Wiley, 2010.
4. Bequette B.W., "Process Control – Modeling, Design and Simulation", Prentice Hall, 2003.
5. Roffel B. and Betlem B., "Process Dynamics and Control-Modeling for Control and Prediction", Wiley, 2006.

### **CML 506: Process Analysis, Simulation and Design**

**[(3-0-0); credits:3]**

**Objective:** To train students on advances in process, simulation and design of chemical engineering processes.

**Syllabus:** Introduction to Modelling and Simulation, Steady State Simulation, Definition, Features, Application, Advantages and Limitation of Simulation based Process Design, Dynamic Simulation, Definition, Features, Application, Advantage and Limitations of Dynamic Simulations, Thermodynamics and Phase Equilibria, Physical, Chemical and Thermodynamic Properties of Pure Components and Mixture, Temperature Dependent Properties, Heat capacity, Viscosity, Density, Thermal Conductivity, Surface tension, Enthalpy, Entropy, Heat of Vaporisation of Liquids, Critical Properties, Reduced Properties, heat of Formation, Gibb's Free Energy, Acentric Factor, Normal Boiling Point, Melting Point, Heat of Fusion, Solubility Parameter, Dipole Moment, Heating Values, Molecular Diameter, Liquid Volume Constant, Vapor Pressure, Antony Vapor Pressure, Rackett Number, Unifac Area /Volume Parameters, Polar Parameter, Wilson Molar Volume, Electrolyte Data ( Simple Anion, Simple Cation, Acid Anion, Oxy-acid anion). Understanding of Physical/chemical/thermodynamic Properties and their application in Process Modelling and Simulation.

Phase Behaviour of Mixtures, Vapor- Liquid, Liquid-Liquid, Vapor-Liquid-Solids Phase equilibrium, Fugacity, Activity and equilibrium, Prediction of Phase Equilibrium. Two Lecture

Equation of States, Peng-Robinson, Benedict-Webb-Rubens-Starling, Grayson-Streed, Maxwell-Bonnett Charts, ESD, SAFT, Soave-Redlich-Kwong, API Soave General etc.

Activity Base Models, (Wilson, Vapor Pressure, NRTL, UNIQUAC, Margules, Hiranuma (HRNM), T. K. Wilson, Regular Solution, PSRK, MSRK, Wilson Salt, UNIFAC VLE, UNIFAC LLE, Modified UNIFAC)

Special System (**Henry's Gas Law, Amine (MEA DEA), Sour Water, SRK, PPAQ, TEG, FLOR:** Flory-Huggins method for polymers, **UPLM:** UNIFAC for polymers)

Introduction to Commercial Process Simulator, Packages, Common Features, Stream and Unit Operation Blocks, Thermodynamic Packages, Unit Operations Specifications, Input Specifications, Running Simulation and Generating Result.

Two Phase Flow Method

Establishing Two Phase Flow Pattern, Wave, Stratified, Annular, Dispersed, Slug and Plug Flow in Baker's Chart. Design Guide lines on two phase line sizing, Sizing of Vapor Liquid, Liquid-Liquid and Vapor-Liquid-Liquid Separator., Surge Time, Retention Time, Control Time, HLL, and NLL calculations for separator, Sizing of Control Valve and Relief Valve

Relief Rate Calculations for various Scenario including Fire and other block case, Instrumentation /Power failure case etc. API/520, API 521, API 2000, OSHA 1910.106, NFPA-30

Simulating Distillation Columns

Strippers, Rectifier, Analysing Separation Problems, VLE/LLE Plots, Binary Interaction Parameters, manipulating existing data to match simulated result with actual plant/pilot /lab data, Using VLE/LLE Data for Regressing Binary Interaction Parameters, Residual Curve Mapping, Binodal Plots.

Short-cut column and Rigorous Column, Fractionators, various Distillation Algorithms (Inside-out, Newton Rapson, Simultaneous Correction Method for Distillation Column Modelling, Column Optimization (Reflux ratio, Reboiler Duty, Condenser Duty, No. of Stages, Feed Tray Locations)

Simulation of Azeotropic and Extractive Distillation Columns, Homogeneous and Heterogeneous Azeotropic, Process Scheme Design for Azeotropic Distillation and Multi Component Distillation

Batch Distillation, Fundamentals and Simulation, Batch Distillation System Design and Operation Sequencing.

Simulation of Heat Exchangers, Heat Balance, Heat Curve Generation, Property Curve Generation, Sizing of Heat Exchangers, Condensers, Reboilers, Evaporators, TEMA Guide Line, Interpretation of TEMA Data Sheet, Rating of Heat Exchangers

Simulation of Chemical reactors, Gibbs Free Energy Reactor, Conversion Reactor, Kinetic Reactor, Batch reactor, Kinetic Models, User Subroutine for Kinetic Model development in a Commercial Simulation Environment.

Sensitivity and Optimization in Commercial Simulation Package

Theoretical back-ground of Various Numerical methods for Optimization, Generalized Reduced Gradient Method, Simultaneous Quadratic Programming Method (SQP), SQP with Simultaneous Modular.

Development of Block Diagram, Process Flow Diagram, Piping and Instrumentation Diagram, Plant Layout and Elevation Plant, Piping Routing and Piping Isometrics Drawings ( Interpretation )

Cost Estimation and Plant Economics Analysis

Various Capital Cost Estimation Techniques, Project Cost, Equipment Cost, Utilities Cost, Raw material Cost, Revenue, By-Product credit, Construction Cost, Depreciation, Interest Cost, labour Cost, Royalty, Laboratory Cost, Cash Flow, IRR and Pay-back period calculations.

Simulation of Refinery Separation Processes, Crude Data Assay Analysis, ASTM D86, TBP, ASTM D1160, ASTM D 2887 and other methods of Petroleum Oil Characterization, Pseudo Component Concept, Property calculations ( API Gravity, Watson Factor, Diesel Index, Motor Octane Number, Research Octane Number, Flash Point, Pour Point, Cloud Point, PONA Analysis.

Simulation and Optimization of FCC main Fractionators, Power Recovery Train of FCC unit.

Alternately any other industrial process plant detailed simulation could be included as project assignment.

Introduction to custom modelling within the frame work of a commercial simulation package and integrating the customized unit peration/thermodynamic package with commercial simulation environment. Developing basic engineering package with economics analysis of any commercial scale process plant including PFD, HMB Conceptual P&ID, Equipment Process Data Sheets, Instrument data Sheets and Control narrative.

#### **References:**

1. Analysis, Synthesis and Design of Chemical Processes (3rd Edition) [Richard Turton, Richard C. Bailie,
2. Wallace B. Whiting, Joseph A. Shaeiwitz]
3. Refinery Process Modelling - Gerald L. Kaes  
International Research Papers

#### **CML 507: Novel Separation Processes**

**[(3-0-0); credits:3]**

**Objective:** To train students on advanced separation processes, thermodynamics of separation operations and equilibrium-based design methods.

**Syllabus:** Introduction to Separation Processes

Thermodynamics of Separation Operations

Separation by phase addition or creation

Equilibrium-based design methods

Multi-component Separations

Separation by barriers and solid agents

Reactive Separations

Hybrid Separations

Case Studies

#### **References:**

1. Separation Process Principles, Seader J. D., Henley E. J., Wiley, 2001, 2<sup>nd</sup> Edition
2. Chemical Engineering Vol. 2, Richardson J. F., Harker J. H., Elsevier, 2002, 5<sup>th</sup> Edition.
3. Natural Extract using Supercritical CO<sub>2</sub>, Mukhopadhyay M., CRC Press, 2000, 1<sup>st</sup> Edition.
4. Membrane Separation Processes, Nath K., Prentice Hall of India, 2008, 1<sup>st</sup> Edition.
5. Bio-separations: Principles and Techniques, Sivasankar B., Prentice Hall of India, 2005, 1<sup>st</sup> Edition.

#### **CMP 508: Analytical and Instrumental Laboratory**

**[(0-0-2); credits:1]**

**Objective:** To train students on analytical and instrumental methods by practical approach

**Syllabus:** Experiments on following topics will be covered:

High performance liquid chromatography (HPLC)

Gas chromatography (GC)

Gas chromatography with mass spectrometry (GCMS)

Fourier Transform infrared (FTIR)

UV-Spectrophotometer

and Other analytical equipments and instruments

**References:**

1. Harris, D.C., "Quantitative Chemical Analysis" W.H. Freeman and company.
2. Bruno, T.J, and Svoronos, P. D. N., "Handbook of Basic Tables for Chemical Analysis", CRC Press
3. McNair, H. M. and Miller, J. M., "Basic Gas Chromatography", Willy and Sons, Inc
4. Palvia D. L., Lampman G. M., Kriz G. S. and Vyvyan J. R., "Introduction to Spectroscopy", Brooks/Cole
5. Snyder L. R, and Krikland J. J., "Introduction to Modern Liquid Chromatography", A Wiley Interscience Publication
6. Skoog D. A., West D. M., Holler F. J. and Crouch S. R., "Fundamentals of Analytical Chemistry", Brooks/Cole
7. Gary. D. Christian, Analytical Chemistry, John Willy and Sons, Inc
8. Willard, H.M., Merit L.L., "Instrumental Methods of Analysis", CBS publishing and Distribution

**CMP 509: Computational and Design Laboratory**

**[(0-0-2); credits:1]**

**Objective:** To train students on computation and design methods by practical approach

**Syllabus:** Computation and Design experiments will be conducted with the help of in-house code and available commercial software such as: CHEMCAD & ASPEN, CFD SOFTWARE (COMSOL), MATLAB, C' LANGUAGE, POLYMATH etc for flash calculations, Distillation Column, CSTR: Reaction Rate Kinetics, Pipe Simulator, Heat Exchanger, Water Purification Reactor, Determining Arrhenius Parameters using Parameter Estimation, NO Reduction in a Monolithic Reactor etc.

**References:**

1. Santosh K. Gupta, Numerical Methods for Engineers, 2<sup>nd</sup> Edition, New Age International (P) Ltd., New Delhi.
2. Steven C. Chapra & Raymond P Canale, Numerical Methods for Engineers, 4th Edition, Tata McGraw Hill, New Delhi.
3. Bruce A. Finlayson, Lorenz T. Biegler, Ignacio E. Grossmann, Mathematics in Chemical Engineering, 2006 Wiley-VCH Verlag GmbH & Co.
4. Gilbert Strang, Linear Algebra and its applications, Harcourt Brace Jovanovich, 1988.

**CMP 510: Advance Separation Laboratory**

**[(0-0-2); credits:1]**

**Objective:** To train students on computation and design methods by practical approach

**Syllabus:** Experiments on following topics will be covered:

Thermodynamics of Separation Processes

Multicomponent Distillation and other separation

Reactive Distillation

Reactive Adsorption

Reactive Crystallization

Reactive Extraction

Hybrid Separation

Membrane Separations

Supercritical Separations etc.

**References:**

1. Separation Process Principles, Seader J. D., Henley E. J., Wiley, 2001, 2nd Edition
2. Chemical Engineering Vol. 2, Richardson J. F., Harker J. H., Elsevier, 2002, 5th Edition.
3. Natural Extract using Supercritical CO<sub>2</sub>, Mukhopadhyay M., CRC Press, 2000, 1st Edition.

4. Membrane Separation Processes, Nath K., Prentice Hall of India, 2008, 1st Edition.
5. Bio-separations: Principles and Techniques, Sivasankar B., Prentice Hall of India, 2005, 1st Edition.

**CMD 509: Project Phase - I**

**[(0-0-6); credits:3]**

**Syllabus:** In this course, the candidate is expected to start his/ her basic preparation of experimental / mathematical project decided by the faculty advisor.

The distribution of marks will be as follows:

- (a) 20% weightage : Proposal / Synopsis of Project
- (b) 10% weightage : Basic preparation for project
- (c) 15% weightage : Presentation and viva -I
- (d) 30% weightage : Final Report
- (e) 25% weightage : Presentation and viva -II

**CMD 510: Project Phase - II**

**[(0-0-18); credits:9]**

**Syllabus:** In this course, the candidate is expected to complete his/ her experimental / mathematical project in continuation of Project Phase – I.

The distribution of marks will be as follows:

- (a) 10% weightage : Proposal / Synopsis of work done in Phase-I and to be done in Phase-II
- (b) 30% weightage : Mide Term Presentation and viva -I
- (d) 30% weightage : Final Report
- (e) 30% weightage : Presentation and viva -II



**List of Elective Subjects (Total credits to be taken = 16)**

<b>Course Code</b>	<b>Course Title</b>	<b>L T P C</b>
CML 521	Chemical Engg. Computational Fluid Dynamics	3 0 0 3
CML 522	Membrane Separation Processes	3 0 0 3
CML 523	Petroleum Engineering	3 0 0 3
CML 524	Polymer Science and Engineering	3 0 0 3
CML 525	Catalysis: Theory and Practice	3 0 0 3
CML 526	Total Quality Management	3 0 0 3
CML 527	Mineral Beneficiation	3 0 0 3
CML 528	Interfacial Science and Engineering	3 0 0 3
CML 529	Optimization Techniques in Process Design	3 0 0 3
CML 530	Process Intensification	3 0 0 3
CML 531	Environmental Management Systems	3 0 0 3
CML 532	Energy Technology and Conservation	3 0 0 3
CML 533	Mass Transfer with Chemical Reaction	3 0 0 3
CML 534	Reliability Analysis in Process Industry	3 0 0 3
CML 535	Advanced Nanotechnology	3 0 0 3
CML 536	Analysis and Design of Experiments*	3 0 0 3
CMP 541	Advance Chemical Process Laboratory	0 0 2 1
CMP 542	Advance Process Simulation Laboratory	0 0 2 1

**CML 521: Chemical Engineering Computational Fluid Dynamics****[(3-0-0); credits:3]**

**Objective:** Provide students with basic understanding of applied computational fluid dynamics (CFD). To teach students to solve a fluid flow problem using different numerical techniques available for CFD. To teach students to apply CFD techniques for simulation of practical problems in fluid flow / heat transfer.

**Syllabus:** Introduction to Computational Fluid Dynamics (CFD) and modelling of flow; Summary of governing equations; Conservation form of equations; Well-posed and ill-posed problems.

Discretisation of the equations; Truncation and Round-off error; Explicit and Implicit approaches; Concepts of numerical or artificial viscosity; Different boundary conditions.

Application of Finite Difference methods to Steady-state problems, One dimensional heat conduction transfer through a pin-fin, Two dimensional conduction through a plate unsteady state problem, One dimensional transient heat conduction, Explicit and implicit methods, Assessing accuracy and stability of numerical methods.

Numerical methods for boundary layer type equations, Navier-Stokes equations, Outline of MAC and SIMPLE algorithms.

Solution of Flow with coupled heat transfer (forced and natural convection); Outline of Reactive flow (combustion) and multi-phase flow. Introduction of a commercial CFD package, CFD case studies: Design of stirred tank reactor, heat transfer in rotary kiln reactors, heat transfer in pyrolysis of biomass particle, etc.

**References:**

1. P. S. Ghoshdastidar, Computer simulation of flow and heat transfer, Tata McGraw-Hill Publishing, 1<sup>st</sup> Edition, 1998.
2. K. Muralidhar and T. Sundararajan, Computational fluid flow and heat transfer, Narosa Publications, 2<sup>nd</sup> Edition, 2003.
3. H. K. Versteeg and W. Malalasekera, An introduction to CFD, Longman Scientific and Technical, 1<sup>st</sup> Edition, 1995.
4. E. S. Oran and J. P. Boris, Numerical simulation of reactive flow, Cambridge University Press, 2<sup>nd</sup> Edition, 2001.
5. J. H. Ferriger, M. Peric, Springer, Computational methods for fluid dynamics, 1<sup>st</sup> Edition, 1996.
6. S. V. Patankar, Numerical heat transfer and fluid flow, Mc Graw-Hill Book Company, 1<sup>st</sup> Edition, 1980.
7. W. Rodi, Turbulence models and their applications – a state of the art review, IAHR – AIRH Monograph series, 3<sup>rd</sup> Edition, 1993.

**CML 522: Membrane Technology****[(3-0-0); credits:3]**

**Objective:** To train students on membrane preparation, membrane characterization, module and process design, application of membrane.

**Syllabus:** Introduction: Separation process, Introduction to membrane processes, classification of membrane processes.

Preparation of Synthetic Membranes: Types of Membrane materials, preparation of Synthetic membranes, phase inversion membranes, preparation technique for immersion precipitation, and preparation technique for composite membranes.

Characterization of Membranes: Introduction, membrane characterization, characterization of porous membranes, characterization of non-porous membranes. Transport in Membranes: introduction, driving forces, non equilibrium thermodynamics, transport through porous, nonporous, and ion exchange membranes.

Science and technology of microfiltration, reverse osmosis, ultrafiltration, nanofiltration, dialysis and electro dialysis, pervaporation, liquid membrane permeation, gas separation, membrane reactors.

Polarization Phenomenon and Fouling: Introduction to concentration polarization, turbulence promoters, pressure drop, gel layer model, osmotic pressure model, boundary layer resistance model, concentration polarization in diffusive membrane separations and electro dialysis, membrane fouling, methods to reduce fouling, compaction.

Module and Process Design: Introduction, plate and frame module, spiral wound module, tubular module, capillary module, hollow fiber module, comparison of module configurations.

Applications and case studies on various membrane separation plants e.g. dehydration of ethanol, sea water desalination.

**References:**

1. Basic Principles Of Membrane Technology, second edition, Marcel Mulder, Springer (India) private limited, 2007.
2. Separation Process Principles:Chemical And Biochemical Operations, J.D.Seader, Ernest J. Henley, D. Keith Roper, 3<sup>rd</sup> edition, Wiley 2010.
3. Membrane Separation Processes, Nath K., Prentice Hall of India, 2008, 1<sup>st</sup> Edition

**CML 523: Petroleum Engineering**

**[(3-0-0); credits:3]**

**Objective:** To train students in petroleum engineering and biorefinery concept.

**Syllabus:** Composition of petroleum, refinery products, characterization of crude oil. Design of crude oil distillation column.

Secondary conversion processes: Catalytic cracking. Catalytic reforming. Delayed coking. Furnace design.

Hydrogenation and Hydrocracking, Isomerization, Alkylation and Polymerization.

Lube oil manufacturing: Lubricating oil, grease and Bitumen

Energy conservation in petroleum refineries. New Trends in petroleum refinery operations, Biorefinery concept

**References:**

1. Modern Petroleum Refining Processes,Bhaskara Rao B.K,Oxford & IBH Publishing Co. Pvt. Ltd. New Delhi,Edition 3<sup>rd</sup>
2. Petroleum Refining Engineering,Nelson W.LTata McGraw Hill Publication Co. Ltd. (1985),4<sup>th</sup> Edition
3. Modern Petroleum Technology,Hobson G.D. & Rohl W.,Applied Science Publication,4<sup>th</sup> Edition
4. Petroleum Refining Technology and Economics,Gary J.H. & Handwerk G.E.,Marcel Dekker, Inc., New York,3<sup>rd</sup> Edition
5. Petroleum Refining Manual,Noel H.M.,Publisher Reinhold Pub. Corp., New York
6. Petroleum Refining Technology,Ram Prasad,Khanna Publishers

**CML 524: Polymer Science & Engineering**

**[(3-0-0); credits:3]**

**Objective:** To train students on polymer processing, testing of polymers, management and recycling of polymers.

**Syllabus: Introduction:** Comparison of thermoplastics and thermoset plastics; Thermoset plastics - Types of resins, Interpenetrating Polymer Networks (IPN); Thermoplastics - Types of aliphatic and aromatic thermo plastics, copolymers, Blends and alloys; Liquid crystal plastics; cellular plastics; oriented plastic materials.

**Processing:** Basics of process design, Classification & general aspects of processes - molding & forming operations, Post die processing; Decoration of plastics - Printing, Vacuum Metalizing, In-mold decoration. Additives & Compounding - Different types of additives, Batch mixers, continuous mixers, Dispersive and distributive mixing, Characterization of mixed state.

Fundamentals on Viscous & Viscoelastic behavior of polymer melt, Rheological measurements and Polymer processability. Non isothermal aspects - Temperature effect on rheological properties, Crystallization, Morphology & Orientation, plastic memory, Molecular weight effects on processing and properties.

**Properties & Testing of plastics:** Basic concepts of testing, National & International standards, Test specimen preparation, Pre conditioning & Test atmosphere.

Identification of plastics by simple test - Visual examination, Density, Melting point, Solubility test, Flame test, Chemical tests.

Effect of shape & structure on material properties, Long - term & short - term mechanical properties, crazing, Permeability & barrier properties, Environmental-stress cracking, Melt flow index, Heat

deflection temperature, Vicat softening temperature, Glass transition temperature, thermal conductivity, Co-efficient of thermal expansion, Shrinkage, Thermal stability, Flammability.

**Waste management & Recycling:** Plastics waste and the associated problems, Integrated waste management - source reduction, recycling & sustainability correlation, energy recovering process. Environmental issues, policies and legislation in India.

### **Kinetics of polymerization (addition and condensation)**

#### **References:**

1. Plastics - How Structure Determines Properties, Gruenwald G, Hanser Publishers, 1993
2. Polymer Processing Principles and Design, Baird D. G. and Collias D. I., Butterworth-Heinemann, 1995
3. Hand Book of Plastics Testing Technology , Vishu Shah, John Wiley & Sons Inc. New York
4. How to identify Plastics by Simple Methods. J.S.Anand, K.Ramamurthy, K.Palanivelu, CIPET, Chennai, 2<sup>nd</sup> edition
5. Plastics and the Environment, Anthony L. Andrady (Ed.), Wiley Interscience, New York

### **CML 525: Catalysis: Theory & Practice**

**[(3-0-0); credits:3]**

**Objective:** To train students on studies in catalysis characterization, diffusion and mass transfer in catalyst, application of film penetration and renewal theories, applications of fluidization technique in process industries

#### **Syllabus:**

Heterogeneous processes. Global rates of reaction. Catalysis. General characteristics of catalysis. Physical adsorption and chemisorption. Adsorption isotherms, Determination of surface area of a catalyst. Classification of catalyst, catalyst preparation. Catalyst deactivation. Langmuir- Hinshelwood and Eley – Rideal model. Rate equation when surface reaction, adsorption and desorption control. External Diffusion effects on heterogeneous catalytic reaction. Modeling diffusion without reaction.

External resistance to mass transfer. Mass transfer limited reaction in packed beds. Diffusion and reaction in porous catalyst pellets. Effective diffusivity and effective thermal conductivity. Internal effectiveness factor. Thiele modules. Mass transfer and reaction in a packed bed reactor. Gas- solid non catalytic reaction –shrinking core model – Diffusion through ash layer, chemical reaction and gas film controls.

Limitation of shrinking core model. Determination of the rate controlling step. Design of gas solid particle reaction. Gas – liquid reaction. Absorption combined with chemical reaction. Mass transfer coefficients and kinetic constants. Application of film penetration and surface renewal theories. Hatta number and enhancement factor for first order reaction. Tower reactor design.

Phenomena of Fluidization, liquid like behavior of fluidized beds, advantages and disadvantages of fluidized beds, different types of fluidized beds and applications of fluidization technique in process industries. Heat and Mass Transfer in Fluidized Beds : Variables affecting heat transfer rate, heat transfer at the wall of containing vessel, heat transfer to immersed tubes. Models proposed by (i) Wicke- Fetting, (ii) Mickley and Fair Banks and (iii) Levenspiel and Walton. Heat transfer in fixed and fluidized beds. Definition and evaluation of mass transfer coefficient.

#### **References:**

1. Smith J.M., Chemical Engineering Kinetics, McGraw Hill
2. Fogler H.S., Elements of Chemical Reaction Engineering, Prentice Hall of India
3. Levenspiel O., Chemical Reaction Engineering, John Wiley
4. Hill C.G., An Introduction to Chemical Engineering Kinetics & Reactor Design, John Wiley
5. B. Viswanathan, S. Sivasanker, A. V. Ramaswamy, Catalysis: Principles and
6. Applications , Academic Press
7. R. A. Van Santen, Piet W. N. M. Van Leeuwen, Jacob A. Moulijn, Bruce A. Averill, Catalysis: An Integrated Approach , Elsevier
8. Diazo Kunii, and Octave Levenspiel, Fluidization Engineering, Butterworth-Heinemann  
Max Leva, Fluidization, McGraw-Hill
9. Carberry J. J., Chemical and Catalytic Reaction Engineering, Courier Dover Publications

### **CML 526: Total Quality Management**

**[(3-0-0); credits:3]**

**Objective:** To train students on studies in TQM, SWOT analysis, failure rate analysis, TQM road map.

**Syllabus:**

Definition of quality-internal and external customers- vision statement – mission statements – objectives – goals – targets- evolution of TQM – Defining TQM – stages in TQM implementation-TQM models  
SWOT analysis-strategic planning-customer focus-quality function deployment-customer satisfaction measurement-seven new management tools-Deming wheel-zero defect concept- benchmarking-six sigma concepts-failure mode and effect analysis-poke yoke

Five S for quality assurance-quality circle philosophy-failure rate analysis-mean failure rate- mean time to failure (MTTF)-Mean time between failure (MTBF)-hazard models-system reliability-availability-maintenance

Quality and cost-characteristics of quality cost-micro analysis of quality cost-measurement of quality-TQM road map- ISO 9000 series certification-ISO 9001:2000 certification-ISO 14000 certification-QS 9000 auditing-Quality auditing- quality awards

**References:**

1. L Suganthi, Anand A Samuel, Total Quality Management, PHI
2. Lt.Gen. Lal H, Total Quality Management, Wiley Eastern Limited
3. Greg Bounds, Beyond Total Quality Management, McGraw Hill Publishers
4. Menon H G, TQM in New Product Manufacturing, McGraw Hill Publishers

**CML 527: Mineral Beneficiation****[(3-0-0); credits:3]**

**Objective:** To train students on advances in mineral beneficiation, sampling methods, power laws, evaluation of particle size, dry and wet classifiers, and flotation principles.

**Syllabus:**

Exploitable characteristics of minerals. Economics of mineral beneficiation. Important beneficiation circuits of minerals like chalcopyrites, sphalerite, galena, bauxite etc.

Different sampling methods and Mechanism and importance of liberation of material.

Power laws. Principles of crushing and grinding. Grindability. Classification, design and application of crushers and grinders..

Evaluation of particle size. Size distribution curves and their significance. Industrial screening, classification and performance of screens.

Dry and wet classifiers. Free and hindered settling, Thickeners, hydro cyclones, filtration, agitation and mixing, tabling, jigging, magnetic and electrostatic separation.

Surface behavior and flotation principles. Flotation machines, differential flotation and flotation circuit design.

**References:**

1. Principles of Mineral Dressing by A. M. Gaudin
2. Principles of Mineral Dressing by Fuerstenau, M. C. and Han, K. N.
3. A Text-Book of Ore Dressing by R. H. Richards
4. Flotation, by A. M. Gaudin
5. Principles of Flotation by K. L. Sutherland and I. W. Wark
6. Mixing Theory and Practice by C. W. Clump and V. W. Uhl.
7. Handbook of Mineral Dressing: Ores and Industrial Minerals by A. F. Taggart.
8. Mineral Processing by Jain

**CML 528: Interfacial Science and Engineering****[(3-0-0); credits:3]**

**Objective:** To train students on concepts of surface and interfacial energies and tensions, mesoscale thermodynamics, mesoscale phenomena in soft matter and applications, and stability of nanoparticle dispersions

**Syllabus: Surface Tension, Adhesion and capillarity:** Effects of confinement and finite size; Concepts of surface and interfacial energies and tensions; A polar (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.

**Intermolecular, nanoscale and interfacial forces in organic, polymeric, biological and aqueous systems:** Van der Waals, Electrostatic double layer, Acid-base interactions including hydrophobic attraction and hydration pressure.

**Mesoscale thermodynamics:** Gibbs treatment of interfaces; concept of excess concentration; variation of interfacial tensions with surfactant concentration.

**Mesoscale phenomena in soft matter and applications:** Adhesion, wetting, nucleation, flotation, patterning of soft material by self-organization and other techniques.

**Stability of nanoparticle dispersions:** DLVO and DLVO like theories and kinetics of coagulation plus general principles of diffusion in a potential field/Brownian movement.

Micellization, Emulsions, Foam, Micro-emulsions.

#### **References:**

1. P.C. Hiemenz, and R. Rajagopalan, Principles of Colloid and Surface Chemistry, 3rd Edition, Marcel Dekker, N.Y., 1997.
2. M.J. Rosen, Surfactants and Interfacial Phenomena, Wiley-Interscience Publication, New York, 2004.
3. A.W. Adamson, A. P. Gast, Physical Chemistry of Surfaces, Wiley-Interscience, New York, 1997.
4. J. Israelachvili, Intermolecular and Surface Forces, Academic Press, New York, 1992
5. D.J. Shaw, Colloid & Surface Chemistry, Butterworth Heinemann, Oxford, 1991.

#### **CML 529: Optimization Techniques in Process Design**

**[(3-0-0); credits:3]**

**Objective:** To train students on identifying the optimization problems, numerical methods for optimizing a function, Linear programming and applications, Optimization of Unit operations, Genetic Algorithms

**Syllabus:** Nature and organization of optimization problems: what optimization is all about, Why optimize, scope and hierarchy of optimization, examples of applications of optimization, the essential features of optimization problems, general procedure for solving optimization problems, obstacles to optimization. Classification of models, how to build a model, fitting functions to empirical data, the method of least squares, factorial experimental designs, fitting a model to data subject to constraints.

Basic concepts of optimization: Continuity of functions, unimodal versus Multimodal functions. Convex and Concave functions, Convex region, Necessary and sufficient conditions for an extremum of an unconstrained function, interpretation of the objective function in terms of its quadratic approximation.

Optimization of unconstrained functions: one-dimensional search:

Numerical methods for optimizing a function of one variable, scanning and bracketing procedures, Newton's, Quasi-Newton's and Secant methods of uni-dimensional search, region elimination methods, polynomial approximation methods, how the one-dimensional search is applied in a multi-dimensional problem, evaluation of uni-dimensional search methods.

Unconstrained multivariable optimization:

Direct methods, random search, grid search, uni-variate search, simplex method, conjugate search directions, Powell's method, indirect methods- first order, gradient method, conjugate method, indirect method- second order: Newton's method forcing the Hessian matrix to be positive definite, movement in the search direction, termination, summary of Newton's method, relation between conjugate gradient methods and Quasi-Newton method.

Linear programming and applications: Basic concepts in linear programming, Degenerate LP's – graphical solution, natural occurrence of linear constraints, the simplex method of solving linear programming problems, standard LP form, obtaining a first feasible solution, the revised simplex method, sensitivity analysis, duality in linear programming, the Karmarkar algorithm, LP applications.

Optimization of Unit operations-1 recovery of waste heat, shell & tube heat exchangers, evaporator design, liquid liquid extraction process, optimal design of staged distillation column.

Optimization of Unit operations-2 Optimal pipe diameter, optimal residence time for maximum yield in an ideal isothermal batch reactor, optimization of thermal cracker using linear programming.

Genetic Algorithms: (Qualitative treatment) Working principles, differences between GAs and traditional methods, similarities between GAs and traditional methods, GAs for constrained optimization, other GA operators, real coded GAs, Advanced Gas

#### **References:**

1. Optimization of Chemical Processes, Edgar, T.F., D.M. Himmelblau, and L.S. Lasdon, McGraw-Hill
2. Engineering Optimization Theory and Practice, Rao, S.S., A Wiley Inetrscience Publication
3. Engineering Optimization: Methods and Applications, Reklaitis, G.V., A. Ravindran, and K.M. Ragsdell, John Wiley
4. Practical method of optimization, Fletcher R., John Wiley
5. An Introduction to optimization, Chong E.K.P. and Zal S. H., John Wiley
6. Numerical Optimization, Nocedal J. and Wright S.J., Springer
7. Genetic Algorithms and Engineering Optimization, G. Mitsuo and C. Runwei, John Wiley

### **CML 530: Process Intensification**

**[(3-0-0); credits:3]**

**Objective:** To train students on advances in to process intensification, reactive and hybrid separations, process synthesis and integration, multifunctional reactors

**Syllabus:** Introduction to Process Intensification: History, Philosophy, principles

High Gravity Fields: process fundamentals, Rotating packed Bed, Design, Applications, Scale-up

Spinning Disc Reactor: mathematical models, heat & mass transfer, design, application

Compact multifunctional heat exchangers: types, applications, design

Microreaction technology: enhancement of heat and mass transfer, control and safety, fabrication, application, design

Structured catalyst and reactors: monolithic reactors, catalysts, gas-phase reactions, application, design

Inline and high intensity mixers: concept of mixing, motionless mixers, mixing and reaction, design, gas-liquid mixing, combined heat exchanger and reactors, design, applications

Reactive and hybrid separations: concept of reactive separations, reactive distillation, membrane based reactive separation reactive adsorption, reactive extraction, reactive crystallization, hybrid separations, extractive distillation, adsorptive distillation, , membrane distillation , membrane chromatographic separation, design, applications

Multifunctional reactors: Concept, integration of reaction, mass and heat transfer, design, application, various equipments,

Process synthesis and integration: conventional design, conceptual design, elements, reaction engineering, complex distillation, systems, industrial studies

Process intensification for industrial safety: concept of industrial safety, hazardous reactions and safety, applications, examples

Industrial practice: methodology and applications, commercial examples of process intensification

#### **References:**

1. Re-engineering the chemical processing plant :process intensification, Andrzej Stankiewicz, JacobA. Moulijn, Marcel Dekker, Inc., Marcel Dekker, Inc., 1<sup>st</sup> edition, 2004
2. Process Intensification in Practice, Cornelis de Weerd, John Wiley and Sons, 1<sup>st</sup> edition, 2005

### **CML 531: Novel Separation Processes**

**[(3-0-0); credits:3]**

**Objective:** To train students on advances in environmental management, environmental impact assessment, environmental audit, and life cycle assessment

**Syllabus:** Environmental management- principles, problems and strategies; Review of political, ecological and remedial actions; future strategies; multidisciplinary environmental strategies, the human,planning, decision-making and management dimensions; environmental impact assessment (EIA), definitions and concepts, rationale and historical development of EIA, sustainable development, Initial environmental examination, environmental impact statement, environmental appraisal, environmental impact factors and areas of consideration, measurement of environmental impact, organization, scope and methodologies of EIA, status of EIA in India; Environmental audit, definitions and concepts, environmental audit versus accounts audit, compliance audit, methodologies and regulations; introduction to ISO and ISO 14000; Life cycle assessment; Triple bottom line approach

#### **References:**

1. R.Welford, Corporate Environmental Management, Earthscan Publications Limited, London, 2002.
2. D. Sayre, Inside ISO 14000 : Competitive Advantage of Environmental Management, St. Louis Press, Florida, 2000.
3. C.S.Rao, Environmental pollution controls engineering, Willey Eastern Ltd., 1991.
4. Materials and Statutes, Tripathi Pvt. Ltd, Bombay, 1992.
5. Deneves, "Air Pollution Control Engineering", Mc .Graw hill, 1999.
6. Jr. W.C. Blackman, "Basic Hazardous Waste Management", CRC Press.
7. K.L. Mulholland, J.A. Dye, "Pollution Prevention: Methodology

### **CML 532: Energy Technology and Conservation**

**[(3-0-0); credits:3]**

**Objective:** To train students on advances in various energy technologies, recent developments in the fields and future challenges, concept of energy

**Syllabus:** Sources of energy, different forms and conversion , solid, liquid and gaseous fuels, composition Analysis, heating values, combustion of fuels, furnaces and furnace streams, material and energy Balance, consumption and heat transfer efficiency, furnace design, oxidation of sulfur and sulfur compounds, alternate sources of energy, energy auditing, case studies, principle of renewable energy, technical and social implications. Solar radiation, measurement and estimation, solar heating devices, solar water heaters, sheltered and unsheltered heaters, systems with separate storage, selective surfaces, solar ponds, solar concentrators and other devices, Bio fuels: classification, combustion and pyrolysis, production of alcohol and bio gas. Bio diesel, fundamentals, transesterification of vegetable oils for bio diesel production, characterization of bio diesel, economics, current trends, future prospects.

Hydrogen energy,: system and analysis, hydrogen infrastructure, safety, codes and standards. Hydrogen production: Electrolysis, thermochemical, hydrogen from fossil fuels, biomass a renewable sources of energy. Hydrogen storage, carbon storage materials, metal and chemical hydrides, cryogenic hydrogen storage, hydrogen fuel cells. Recent developments in the fields and future challenges. Concept of energy

#### **References:**

1. Fuels & Fuel Technology : Francis W; Peter M.C Pergmon Press
2. Fuel Combustion Energy Technology: S.N.Saha, Dhanpat Rai Pub.Co. New Delhi
3. Conventional Energy Technology : S.B.Pandya, Tata McGraw Hill
4. Practical Techniques of Saving Energy in Chemical Industries : Sitting M, Noyes Data Corp. USA.
5. Brame J. S. S. and King J. G. Edward Arnold, " Fuel, Solid, Liquid and Gases"
6. Sukhatme S.P., "Solar Energy"

### **CML 533: Mass Transfer with Chemical Reaction**

**[(3-0-0); credits:3]**

**Objective:** To train students on theory of mass transfer accompanied by irreversible and reversible reactions, discussion and examples of systems falling in different regimes, use of models in the simulation and design of fluid-fluid reactors

**Syllabus:** Introduction to mass transfer and reaction engineering

Theory of mass transfer accompanied by irreversible and reversible reactions of general order; methods of discerning controlling mechanism: Very slow reactions, slow reactions, fast reactions, instantaneous reactions, overlapping of regimes, controlling mechanisms

Discussion and examples of systems falling in different regimes: gas-liquid system, liquid-liquid system, special cases, reversible reactions

Mass transfer accompanied by consecutive and two-step reactions:

Absorption of a gas into a solution containing two reactants:

Simultaneous absorption and reaction of two gases:

Reaction in both (liquid) phases:

Desorption with chemical reaction; simultaneous absorption-desorption with reaction:

Complex reactions:

Use of models in the simulation and design of fluid-fluid reactors

Solid-liquid reactions

#### **References:**



1. Heterogeneous reactions: Analysis, examples, and reactor design. L. K. Doraiswamy and M. M. Sharma, John Wiley and Sons, New York, 1984, Vol. II
2. Chemical Reactor Analysis, G. F. Froment and K. B. Bischoff, John Wiley & Sons, Singapore, 1990 2<sup>nd</sup> Edition.
3. Chemical Reaction Engineering, Octave Levenspiel, John Wiley & Sons, Singapore, 1998 3<sup>rd</sup> Edition.
4. Elements of Chemical Reaction Engineering, Fogler H.S., Prentice-Hall, NJ, 2006, 4<sup>th</sup> Edition
5. Chemical Engineering Kinetics, Smith J. M., McGraw Hill, N Y, 1981, 3<sup>rd</sup> Edition.

### **CML 534: Reliability Analysis in Process Industry**

**[(3-0-0); credits:3]**

**Objective:** To train students on reliability Engineering in process industry, state dependent systems, design for reliability, case Studies in process industries

**Syllabus:** Introduction to probability: review of sets, events, definitions, finite sample spaces and enumeration, conditional probability, partitions theorem, total probability theorem, Bayes' theorem

Reliability Engineering in process industry - Introduction: concept, terms, definitions, applications, history

Failure distribution: Reliability function, MTF, HRF, bathtub curve, conditional reliability

Constant failure rate model: exponential function, failure modes, applications, two-parameter exponential distribution, Poisson process

Time dependent failure models: Weibull distribution, normal distribution, lognormal distribution

Reliability of systems: serial, parallel configuration, SSF, minimal cuts, minimal paths, common-mode failures, three state devices

State dependent systems: Markov analysis, load sharing systems, standby systems, degraded systems, three state devices

Physical reliability models: covariate, static, dynamic models, physics of failure models

Design for reliability: specification and system measurements, reliability allocation, design methods, failure analysis, system safety and fault tree analysis

Maintainability: analysis of downtime, repair time distribution, stochastic point processes, system repair time, reliability under preventive maintenance

Availability: concepts and definitions, models, system availability, design analysis

Data collection and empirical methods

Identifying failure and repair distribution

Case Studies in process industries

#### **References:**

1. Practical Reliability Engineering, O'Connor P. D. T., John Wiley and Sons (Asia) Pvt. Ltd., 4<sup>th</sup> edition, 2002
2. Introduction to Reliability and Maintainability Engineering, Ebeling C. E., Tata McGraw-Hill, New York, 1<sup>st</sup> edition, 5<sup>th</sup> reprint, 2005

### **CML 535: Advanced Nanotechnology**

**[(3-0-0); credits:3]**

**Objective:** To train students on advances in nanotechnology, synthesis of nanoparticles, carbon fullerenes and nanotubes, micro and mesoporous materials, characterization and properties of nanomaterials.

**Syllabus: Introduction to Nanotechnology:** Introduction, Emergence of Nanotechnology ,Bottom-Up and Top-Down Approaches, Challenges in Nanotechnology

Surface Energy, Chemical Potential as a Function of Surface Curvature, Electrostatic Stabilization, Surface charge density, Electric potential at the proximity of solid surface, Van der Waals attraction potential, Interactions between two particles: DLVO theory, Steric Stabilization, Solvent and polymer, Interactions between polymer layers, Mixed steric and electric interactions

**Synthesis of Nanoparticles:** Synthesis of metallic nanoparticles, Influences of reduction, reagents, Influences by other factors, Influences of polymer stabilizer, Synthesis of semiconductor nanoparticles, Synthesis of oxide nanoparticles, Introduction to sol-gel processing, Forced hydrolysis, Controlled release of ions

**Special Nanomaterials:** Introduction

**Carbon Fullerenes and Nanotubes:** Carbon fullerenes, Fullerene-derived crystals, Carbon Nanotubes

**Micro and Mesoporous Materials:** Ordered mesoporous structures, Random mesoporous structures

Crystalline microporous materials: zeolites

**Core-Shell Structures:** Metal-oxide structures, Metal-polymer structures, Oxide-polymer structures

**Characterization and Properties of Nanomaterials:** Introduction, Structural Characterization, X-ray diffraction (XRD), Small angle X-ray scattering (SAXS), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Scanning probe microscopy (SPM), Gas adsorption

**Applications in Engg and Technology:** Application in Nanofluids, Applications in Polymer, Applications in separation technology

**References:**

1. Nanostructures and Nanomaterials (synthesis properties and applications, Guozhong Cap, Ying Wang, World Scientific, 2<sup>nd</sup> Edition, USA 2011
2. Nanotechnology (strategies, industry trends and applications, Jurgen Schulte, Willey, 1<sup>st</sup> Edition, England 2005
3. Carbon Nanotubes (Basic concept and physical property, S.Reich, C.Thomsen, J.Maultzsch, Wiley-VCH
4. 1<sup>st</sup> Edition, 2004, Weinheim.
5. Polymer Rheology theory and practice, Yuri G. Yanovsky, Chapman and Hall, 1<sup>st</sup> Edition 1993
6. Nanostructured Materials, Gerhard Wilde, Elsevier, 1<sup>st</sup> Edition, Netherland, 2009

**CML 536: Analysis and Design of Experiments**

**[(3-0-0); credits:3]**

**Objective:** To train students on advances in different designs, regression approach, parameter design and multivariate analysis of variance.

**Syllabus:** Introduction

Analysis of Variance

Factorial Experiment design

Nested Design

Confounded Design

Regression Approach

Response Surface Methodology

Orthogonal Arrays

Parameter Design

Multivariate Analysis of Variance

**References:**

1. Design and Analysis of Experiments, Douglas C. Montgomery, 8<sup>th</sup> Edition, Wiley
2. Design and Analysis of Experiments, R. Panneerselvam, PHI Learning Private Ltd., 2012
3. A First Course in Design and Analysis of Experiments, Gary W. Oehlert
4. Experimental Design and Analysis, Howard J. Seltman

**CMP 541: Advance Chemical Process Laboratory**

**[(0-0-2); credits:1]**

**Objective:** To train students on advance chemical processes by practical approach

**Syllabus:** In this laboratory, few typical chemicals / compounds will be synthesized, characterized and used for typical application. Further complete process will be studied base on thermodynamics and other chemical engineering aspects.

**References:**

Chemical Process Principles, Seader J. D., Henley E. J., Wiley, 2001, 2nd Edition

Chemical Engineering Vol. 2, Richardson J. F., Harker J. H., Elsevier, 2002, 5th Edition.

**CMP 542: Advance Process Simulation Laboratory**

**[(0-0-2); credits:1]**

**Objective:** To train students on advance process simulations with the help of various chemical engineering softwares.

**Syllabus:** Simple Simulation Cases using any of the Commercial Simulation Software ( Aspen Plus, Hysys, Unisim, Pro II, Chemcad) for Fluid Dynamics (Pump, Compressors, Expander, Pipe, Valve, Control Valve, piping, Flash calculations, Distillations columns stripers, Rectifier, Analysing Separation Problems, VLE/LLE Plots, Binary Interaction Parameters, manipulating existing data to match simulated result with actual plant/pilot /lab data, Using VLE/LLE Data for Regressing Binary Interaction Parameters, Residual Curve Mapping, Binodal Plots.

Simulation of Chemical reactors Gibbs Free Energy Reactor, Conversion Reactor, Kinetic Reactor, Batch reactor, Kinetic Models, etc. Detailed Simulation of Batch reactor CSTR and Plug Flow reactor with simultaneous Reaction and Heat/Mass Transfer. Commercial Batch reactor and Impeller Design, Design of External Jacket, Internal Coil, Limped Coil.

Steady State Simulation and Optimization using Aspen Plus e.g. Flash Drum Examples, Aspen Plus Simulation of Reactor Models, Aspen Plus Simulation of Distillation Models, Chemical Plant Simulation using Aspen Plus, Introduction, Aspen Plus Simulation of a Distillation Train, Aspen Plus Simulation of Vinyl Chloride Monomer (VCM)

**References:**

1. Analysis, Synthesis and Design of Chemical Processes (3rd Edition) [Richard Turton, Richard C. Bailie, Wallace B. Whiting, Joseph A. Shaeiwitz]
2. Refinery Process Modelling - Gerald L. Kaes