

M.Tech in Chemical Engineering (Specialization: Petroleum Science and Technology)

Semester – 1						Semester - 2					
Course	Course Name	L	T	P	C	Course	Course Name	L	T	P	C
CL 501	Advanced Transport Phenomena	3	0	0	6	CL 503	Advanced Thermodynamics	3	0	0	6
CL 502	Computer Aided Numerical Methods	2	1	2	8	CL 504	Advanced Reaction Engineering	3	0	0	6
CL 511	Petroleum Reservoir Engineering	3	0	0	6	CL 598	Petroleum Laboratory	0	0	3	3
CL 512	Petroleum Refinery Engineering	3	0	0	6	CL 505	Petroleum Production Engineering	3	0	0	6
CL 6XX	Elective I	3	0	0	6	CL 599	Scientific Communications	0	0	2	2
						CL 6XX	Elective II	3	0	0	6
Total Credits		14	1	2	32	Total Credits		12	0	5	29
Semester – 3						Semester - 4					
Course	Course Name	L	T	P	C	Course	Course Name	L	T	P	C
CL 698	Project I	0	0	24	24	CL 699	Project II	0	0	24	24
Total Credits		0	0	24	24	Total Credits		0	0	24	24

M.Tech in Chemical Engineering (Specialization: Materials Science and Technology)

Semester – 1						Semester - 2					
Course	Course Name	L	T	P	C	Course	Course Name	L	T	P	C
CL 501	Advanced Transport Phenomena	3	0	0	6	CL 503	Advanced Thermodynamics	3	0	0	6
CL 502	Computer Aided Numerical Methods	2	1	2	8	CL 504	Advanced Reaction Engineering	3	0	0	6
CL 513	Characterization of Materials	2	0	2	6	CL 514	Fundamentals of Material Science & Engineering	3	0	0	6
CL 6XX	Elective I	3	0	0	6	CL 506	Smart Materials	3	0	0	6
						CL 599	Scientific Communications	0	0	2	2
						CL 6XX	Elective II	3	0	0	6
Total Credits		10	1	4	26	Total Credits		15	0	2	32
Semester – 3						Semester - 4					
Course	Course Name	L	T	P	C	Course	Course Name	L	T	P	C
CL 698	Project I	0	0	24	24	CL 699	Project II	0	0	24	24
Total Credits		0	0	24	24	Total Credits		0	0	24	24

Note: Two specializations will have different sets of elective courses

Pool of Electives	
Course No.	Course Name
CL 611	Advanced Process Control
CL 612	Colloid and Interface Science
CL 613	Computational Fluid Dynamics
CL 614	Fluidization Engineering
CL 615	Optimization Techniques
CL 617	Petrochemicals
CL 618	Natural Gas Engineering
CL 619	Refinery Process Design
CL 620	Nonlinear Bifurcation Analysis
CL 621	Fuel Cell Technology
CL 622	Molecular Simulation: Principles and Application
CL 623	Polymer Science and Technology
CL 624	Computing in Chemical and Petroleum Engineering
CL 625	Fundamentals of micro-nano fluidics & microfabrication
CL 626	Energy Resources
CL 627	Multiphase Flow
CL 628	Catalysts and Adsorbents
CL 629	Membranes
CL 630	Composite Materials
CL 631	Smart Materials
CL 632	Integration of Refinery and Petrochemical Operations
CL 633	Applied Statistical Thermodynamics
CL 634	Applied Rheology
CL 635	Advanced Clean Fuel Technologies
CL 636	Microelectronic Fabrication
CL 637	Multicomponent Mass Transfer (MMT)
CL 638	Mathematical Methods in Chemical Engineering
CL 639	Biofluid Mechanics
CL-641	Process Intensification and Integration
CL 642	Advanced Flow Measurement Techniques
CL 643	Computer Aided Applied Optimization
CL 644	Petroleum Reservoir Simulation
CL 645	Applied Statistics for Chemical Engineers

CL 501	Advanced Transport Phenomena	(3-0-0-6)
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Preamble:

Chemical Engineers, in the undergraduate level, study individually and extensively the subject momentum, heat and mass transfer. They are also exposed to the unified approach of the above transports through a course transport phenomena. Transport of momentum, heat and mass are almost inevitable in every field of engineering sciences including the emerging areas like biotechnology, nanotechnology, microfluidics, microelectronics. Therefore, the postgraduate students must possess detailed and up to date knowledge on transport phenomena through a course named advanced transport phenomena. This would help them to cope up with the industrial and/or research requirements in future.

The course on advanced transport phenomena would first refresh the students on analogical behaviour of the three forms of transport, principles and applications of Reynolds Transport theorem and Navier- Stokes equation. It would then cover various aspects like non-Newtonian flow, turbulent flow, and boundary layer analysis. It would take up cases of simultaneous heat mass and momentum transport and discuss mathematical methods of solution for such transport problems.

Course Contents:

Molecular transport mechanisms and general properties; analogies amongst momentum, heat, and mass transport; non-Newtonian fluids and rheological behaviour; equation of change for isothermal and non-isothermal systems; review of Reynolds Transport theorem and Navier- Stokes equation with applications to flow of Newtonian and non-Newtonian fluids through various devices and under various flow conditions; turbulent flow analysis; boundary layer analysis for momentum, heat, and mass transfer; heat and mass transfer with chemical reaction; mathematical methods for solution of transport equations.

Texts/References:

1. W.M.Deen, Analysis of Transport Phenomena, Oxford University Press, New York, 1998 (First Indian Edition, 2008).
2. B. R. Bird, E. W. Stewart and N. E. Lightfoot, Transport Phenomena, 2nd Ed., John Wiley & Sons, 2003.
3. J. C. Slattery, Advanced Transport Phenomena, Cambridge University Press, 1999.
4. R. E. Treybal, Mass Transfer Operations, 3rd Ed., McGraw-Hill International Edition, 1981.
5. E. L. Cussler, Diffusion: Mass Transfer in Fluid System, Cambridge University Press, 1997.
6. J. P. Holman, Heat Transfer, 8th Ed., McGraw-Hill, 1997.
7. R. W. Fox and A. T. McDonald, Introduction to Fluid Mechanics, 5th Ed., John Wiley & Sons, 1998.

CL 502

Computer Aided Numerical Methods

(2-1-2-8)

Preamble:**Course Contents:**

Course Content/Syllabus: Solution of linear system of equations; nonlinear algebraic and transcendental equations; Curve fitting: linear and non-linear regression; Statistical Aspects of Least Squares Theory; Statistical Distributions; Hypothesis Testing; Analysis of Variance; Solution of non-stiff ordinary differential equations: Initial and boundary value problems; Stiff differential equations; Solution of partial differential equations: Parabolic, elliptic and hyperbolic partial differential equations. Programming of numerical techniques on Computers.

Texts/References:

1. S. C. Chapra and R. P. Canale, Numerical Methods for Engineers, McGraw-Hill Education, 2015
2. P. Ghosh, Numerical Methods with Computer Programs in C++, Prentice-Hall of India Private Ltd., 2006
3. J. H. Mathews and K. D. Fink, Numerical Methods Using MATLAB, 4th Edition, Pearson, 2004
4. S. C. Chapra, Applied Numerical Methods with MATLAB for Engineers and Scientists, 3rd Edition, 2012
5. P. Ghosh, Numerical, Symbolic and Statistical Computing for Chemical Engineers Using MATLAB, Prentice-Hall of India Private Limited, 2018
6. S. K. Gupta, Numerical Methods for Engineers, 3rd Edition, New Age International, 2015.
7. W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Numerical recipes in FORTRAN
8. FORTRAN: the art of scientific programming, Cambridge University Press, 1992

CL 503	Advanced Thermodynamics	(3-0-0-6)
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Preamble:

An important requirement for the design of chemical engineering processes lies in the composition of multiple equilibrium phases. The predictions of these phases involve thermodynamics and its modelling. This course initially encompasses the basic concepts such as fugacity, excess functions and activity. Thereafter the various phase equilibria problems such as Vapour Liquid Equilibria (VLE), Liquid Liquid Equilibria (LLE) and Solid Liquid Equilibria (SLE) are modelled using excess Gibb's free energy models. Advanced topics such as Vapour Liquid Liquid Equilibria (VLLE) and Phase Equilibria of Solid-Solid Mixtures is also demonstrated.

The course has been modified taking into account the two upcoming M. Tech streams i.e. Petroleum Science and Technology and Material Science and Technology. Some key topics such as "Solubility of gases and solids in liquids; High pressure equilibria" has been replaced by topics such as "Solid Liquid Equilibria (SLE); Vapour Liquid Liquid Equilibria (VLLE) and Phase Equilibria of Solid-Solid Mixtures". VLLE and SLE are frequently encountered in petroleum industries. For e.g. Benzene-water solution shows VLLE phenomena at 498.15 K. Similarly, the thermodynamics of waxes and asphaltenes show SLE behaviour. In a same manner, Solid Solid phase mixtures are mostly observed for Material Science Applications.

Course Contents:

Thermodynamics of phase equilibria; Estimation of thermodynamics properties; Fugacity of gas and liquid mixtures; Excess Functions; Calculation of vapour liquid equilibria using equations of state; Classical and excess free energy based mixing rules; Theories of solutions; Liquid models with special emphasis on NRTL, UNIQUAC and UNIFAC theories; Solid-Liquid Equilibria (SLE); Vapour-Liquid-Liquid Equilibria(VLLE); Phase Equilibria of Solid-Solid Mixtures.

Texts/References:

1. J. M. Prausnitz, R. N. Lichtenthaler and E. G. de Azevedo, Molecular Thermodynamics of Fluid-Phase Equilibria, Prentice-Hall, 1999.
2. S. I. Sandler, Chemical, Biochemical and Engineering Thermodynamics, 4th Ed., Wiley India, 2006.
3. J. M. Smith, H. C. V. Ness and M.M. Abbott, Introduction to Chemical Engineering Thermodynamics, McGraw Hill, 2003.
4. A. Firoozabadi and F. Abbas, Thermodynamics of Hydrocarbon reservoirs, McGraw-Hill Professional Publishing, 1999.
5. T. Letcher, Chemical Thermodynamics for Industry, Royal Society of Chemistry, London, 2004.

CL 504	Advanced Reaction Engineering	(3-0-0-6)
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Preamble:

Sound knowledge in advanced reaction engineering is very important for Chemical Engineers. This course would enable students to gain knowledge with respect to various significant industrial reactor configurations including catalytic packed bed reactors, trickle bed reactors, slurry reactors and fluidized bed reactors. Subsequent modelling aspects along with applicable mathematical analysis is eventually presented all along the course. Therefore, the revised syllabus is presented more systematically to what was presented previously with certain modifications.

Course Contents:

Homogeneous reactions; Ideal reactors; Residence Time Distribution (RTD); Non-ideal reactors: Dispersion model; Tank-in-series model; Heterogeneous catalytic reactions; Catalyst deactivation; Design of catalytic reactors: Packed Bed Reactor, Trickle bed reactor, Slurry reactor, Fluidized bed reactor; Non-catalytic fluid-solid reactions: Kinetics and Reactor design; Fluid- fluid reaction kinetics and reactor design.

Texts/References:

1. H. S. Fogler, Elements of Chemical Reaction Engineering, 4th Ed., Prentice-Hall India, 2005.
2. O. Levenspiel, Chemical Reaction Engineering, 3rd Ed., John Wiley, 1999.
3. J. M. Smith, Chemical Engineering Kinetics, 3rd Ed., McGraw-Hill, 1981.
4. J.B. Butt, Reaction Kinetics and Reactor Design, 2nd Ed., Marcel and Dekker, 2000.
5. G. F. Froment, K. B. Bischoff and J. De Wilde, Chemical Reactor Analysis and Design, 3rd Ed. Wiley-VCH, 2010.
6. E.B. Nauman and B.A. Buffham, Mixing in Continuous Flow System, John Wiley & Sons, 1983.
7. E.B. Nauman, Handbook of Chemical Reactor Design, Optimization and Scaleup, MGH publication, 2001.

CL 505	Petroleum Production Engineering	(3 0 0 6)
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Syllabus:

Oil and gas production facilities; Well completion techniques; Well production problems and mitigation; Oil, Water and gas separation systems; Crude Oil treating; Formation damage, Well stimulation techniques, Artificial lift techniques; Field processing of oil & gas; Storage and transportation of petroleum and petroleum products; Production system analysis & optimization; Production testing; Multiphase flow in tubing and flow-lines; Nodal system analysis; Offshore well completion; Deep water applications of subsea technology; Offshore production: Oil processing platforms, water injection platforms, storage, transportation and utilities; Deep water production system.

Text /Reference Books:

1. Surface Production Operations, Ken Arnold & Maurice Stewart, 3rd Edition, Gulf Professional Publishing, 2008.
2. Petroleum and Gas Field Processing, H.K. Abdel- Aal, Mohamed Aggover, M.A. Fahim, Marcel Dekkar Inc., 2003.
3. Offshore Petroleum Drilling and Production, Sukumar Laik, CRC Press, 2018.
4. Oil Well Stimulation, Robert S. Schechter, Prentice Hall, 1992.
5. Modern Fracturing Enhancing Natural Gas Production, Michael J. Economides, Tony Martin, ET Publishing, 2007.
6. Subsea Engineering Handbook, Yong Bai and Qiang Bai, Gulf Professional Publishing, New York, 2012.
7. Petroleum Production Engineering: A Computer Assisted Approach, Boyun Guo, William C. Lyons, Ali Ghalambor, Elsevier Science & Technology Books, 2007.
8. Petroleum Production Systems, M.J. Economides, A. Daniel Hill and C. E. Economides, Prentice Hall, 1994.

CL 506	Smart Materials	(3-0-0-6)
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Preamble:

The objective of this course is to develop the knowledge and awareness of smart materials and concepts to engineering application areas. Students will acquire a critical understanding of mechanisms giving rise to the characteristic and beneficial properties of smart materials. The recent state-of-art on the technological applicability and limits of smart materials will be discussed. The course will provide a basis of understanding for many of the materials and material systems that underlie the analysis and design of "smart" devices.

Course contents:

Introduction to smart materials: definition, type, properties and examples; Modelling of mechanical and electrical system: fundamental relationships in mechanics and electrostatics, work and energy; Mathematical representations of smart material system: first order and second order dynamic systems, frequency response; Piezoelectric materials, shape-memory materials, conductive polymers, pH and temperature sensitive polymer; Engineering and scientific applications of different smart materials, their preparation, characterization and use as smart products; Smart membrane, smart healable materials and chromogenic smart material; Biologically and field responsive smart materials; Applications of different smart materials.

Texts/References:

1. D. J. Leo, Engineering Analysis of Smart Materials Systems, Wiley, 2007.
2. M.V. Ghandi and B.S. Thompson, Smart Materials and Structures, Chapman & Hall, 1992.
3. A.V. Srinivasan and D.M. McFarland, Smart Structures, Cambridge University Press, 2001.
4. H. Janocha (Ed.), Adaptronics and Smart Structures, Springer, 1999.
5. R.C. Smith, Smart Material Systems: Model Development (Frontiers in Applied Mathematics), SIAM, 2005.

CL 511	Petroleum Reservoir Engineering	(3-0-0-6)
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Preamble:

Petroleum reservoir engineering encompasses the application of fundamentals associated to fluid mechanics, geology, hydrocarbon phase behaviour etc. for the safe and efficient operation of petroleum reservoirs. Firstly, the course teaches Origin and occurrence, exploration, recovery and transportation of crude oil. Eventually, the course provides a broad outline with respect to both basic and advanced topics in the field of petroleum reservoir engineering including enhanced oil recovery. Finally, reservoir simulation, natural gas engineering and gas hydrates are also covered to broaden the scope of student learning in this subject. With this approach, the revised syllabus is broad enough to include all basic and advanced topics of petroleum reservoir engineering.

Course contents:

Origin and composition of petroleum; Petroleum geology; Oil well drilling methods; Reservoir rock and fluid properties; Material balance in oil and gas reservoirs; fundamentals of oil and gas flow in porous media, General equation for radial flow of oil and gas in reservoirs, Oil and gas well testing methods; Predicting reservoir performance; Enhanced oil recovery: Water flooding, Polymer and caustic flooding, Surfactant flooding, Microbial enhanced oil recovery and thermal recovery methods; Introduction to Reservoir Simulation; Natural gas and Gas hydrates.

Texts/References:

1. R.E. Terry, M. Hawkins and B.C. Craft, Applied Petroleum Reservoir Engineering, Prentice Hall, 1991.
2. L.P. Dake, Fundamentals of Reservoir Engineering, Elsevier, 1983.
3. T. Ahmed and P. McKinney, Advanced Reservoir Engineering, Elsevier, 2004.
4. G.L. Chierici, Principles of Petroleum Reservoir Engineering, Springer-Verlag, 1994.
5. D.L. Katz and R.L. Lee, Natural Gas Engineering, McGraw-Hill, 1990.

CL 512	Petroleum Refinery Engineering	(3-0-0-6)
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Preamble:

The objective of this course is to understand the chemistry and processes involved in converting the crude oil into valuable products in the petroleum refinery. In addition, the students will gain knowledge with respect to the effects of process variables such as reaction temperature, pressure, space velocity and types of catalyst, etc. on the properties of the products, yield and selectivity. Hydrogen production processes and sulphur recovery processes will also be taught as a part of catalytic reforming and hydro treating process respectively.

Course contents:

Characterization of crude oil and refinery products; crude distillation process: atmospheric distillation unit (ADU), vacuum distillation unit (VDU); Thermal and Catalytic cracking; Catalytic reforming; Hydro treating and Hydrocracking; Light end processes: alkylation, isomerization and polymerization; Heavy end processes: coking, vis-breaking, deasphalting and dewaxing; Lube oil base stock (LOBS) production.

Texts/References:

1. J. H. Gary and G. E. Handwerk, Petroleum Refining: Technology and Economics, 4th Ed., Marcel Dekker, 2001.
2. D.S.J. Jones and P. R. Pujadó, Handbook of Petroleum Processing, Springer, 2006.
3. C.S. Hsu and P. R. Robinson, Practical Advances in Petroleum Processing, Springer, 2006.
4. J. G. Speight and B. Ozum, Petroleum Refining Process, Marcel Dekker, 2002.

CL 513

Characterization of Materials

(3-0-2-8)

Preamble:

Information on the various properties of Materials are the key to unlock and analyse their suitability for various futuristic applications. The course Characterization of Materials aims to address these aspects fundamentally and practically. The study span during the course includes the fundamental principles of various instrumentation techniques which include microscopy, spectroscopy, surface characterization, and the thermal and mechanical stability. After the theoretical exposure, the students are expected to undergo hands-on laboratory experiments to map their fundamental understanding learned to the experimental methods for characterizations. Upon successful completion of the course, students are expected to be conversant with various characterization techniques including characterization of bio/nanostructures and nano/bio/smart materials. They are expected to become competent in carrying out analysis on the structural, thermal, chemical and mechanical properties of materials.

Course contents:

Class Room Components: A. Materials Characterization: Principles of X-ray diffraction (XRD); Chemical analysis by XRD & Fluorescence; Particle size analysis (LPSA)– ζ - potential; Small angle X-ray scattering (SAXS); Introduction to spectroscopy (UV-vis, IR and Raman); X-ray photoemission spectroscopy (XPS); Atomic Absorption Spectroscopy (AAS); Inductively coupled plasma mass spectrometry (ICP-MS); Thin-layer/Ion- exchange/Gel-permeation chromatography (TLC/ILC/GPC); Gas-liquid-partition/high- performance liquid chromatography(HPLC); Gas chromatography (GC); Thermo- gravimetric analysis (TGA)- HPTGA; Differential scanning calorimetry (DSC). B. Mechanical Characterisation: Principles and characterization of tensile, compressive, hardness, fatigue, and fracture toughness properties; Rheology and Rheometers. C. Morphological Characterization: Optical microscopy; Atomic force microscopy (AFM) and Scanning tunneling microscopy (STM); Scanning (SEM) and Transmission electron microscopes (TEM). D. Surface Characterization: BET surface area analysis; chemisorption; Tensiometers – Surface/Interfacial tension.

Laboratory Components: Hands on Experiments on UV-vis and IR spectroscopies; TGA – HPTGA; DSC; BET surface area analyser; ζ -potential analyser – LPSA; Rheometers; Tensiometers; HPLC, GPC and GC with mass spectrometry (GC-MS); AAS; ICP-MS; Porosimetry; Mechanical and thermal analyses.

Texts/References:

1. Y. Leng, Materials Characterization: Introduction to microscopic and spectroscopic methods Ed., John Wiley & Sons, 2008.
2. A.W. Adamson and A.P. Gast, Physical Chemistry of Surfaces, John Wiley, New York, 1997.
3. A.J. Milling, Surface Characterization Methods: Principles, techniques & applications, Marcel Dekker, 1999.
4. W.D. Callister (Jr.), Material Science and Engineering: An Introduction, 8th Ed. John Wiley & Sons, 2010.
5. William D. Callister, Fundamentals of Materials Science and Engineering: An Interactive, 5th Edition, John Wiley & Sons, 2005.
6. David B. Williams, C. Barry Carter, "Transmission Electron Microscopy: A Textbook for Materials Science", Springer 2009.
7. Laboratory Manuals for analysis.

CL 514

Fundamentals of Material Science & Engineering

(3-0-0-6)

Preamble:

Information on a synthesized material remains incomplete unless it is thoroughly analysed to understand its various characteristics and its suitability in desired applications. The course Characterization of Materials is aimed at such target. It is a combined course of both lecture and laboratory components. The fundamental principles of various instrumentation techniques viz. microscopy, spectroscopy, surface characterization, thermal stability analysis and mechanical stability analysis for synthesized materials will be discussed through this course. The students will be exposed to real hands-on laboratory experiments to impart the knowledge of experimental methods for characterization of various synthesized materials. Upon successful completion of this course, students are expected to be conversant with various characterization techniques and will be competent to carry out such experiments in future endeavours to find out the structural, thermal, chemical and mechanical properties of materials of concern.

Course contents:

Materials characterization: importance and applications; principles of X-ray diffraction (XRD) methods; microscopy techniques: optical and electrons (SEM and TEM) microscopy; Introduction to spectroscopy (UV-vis, IR and Raman); thermal stability analysis: thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC); mechanical property characterisation: principles and characterization of tensile, compressive, hardness, fatigue, and fracture toughness properties; principles of characterization of other materials properties: BET surface area; chemisorption; particle size; zeta potential; rheology; and interfacial tension

Texts/References:

1. Y. Leng, Materials Characterization: Introduction to microscopic and spectroscopic methods, 1st Ed., John Wiley & Sons, 2008.
2. A.W. Adamson and A.P. Gast, Physical Chemistry of Surfaces, John Wiley, New York, 1997.
3. D.G. Baird and D.I. Collias, Polymer Processing Principles and Design, Butterworth-Heinemann, Massachusetts, 1995.
4. A.J. Milling, Surface Characterization Methods: Principles, techniques, and applications, Marcel Dekker, 1999.
5. G. Ertl, H. Knozinger and J. Weitkamp, Handbook of Heterogeneous Catalysis, Vol. 2, Wiley- VCH, 1997.
6. W.D. Callister (Jr.), Material Science and Engineering: An introduction, 8th Ed., John Wiley & Sons, 2010.
7. Laboratory Instruction Manual

CL 598	Petroleum Laboratory	(0-0-3-3)
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Preamble:**Course Contents:**

Petroleum product Characterizations: Determination of flash point, smoke point, and fire point etc. of the petroleum products, petroleum products, Detection of contamination of gasoline and diesel, ASTM Distillation, Measurement of petroleum product viscosities etc.; Upstream and downstream experiments: Pressure drop Measurements, Steam distillation; Upstream and downstream simulation through software packages.

Texts/References:

1. G. G. Speight, Handbook of Petroleum Analysis, 1st Ed., John Wiley & Sons, 2001
2. Manuals associated to various petroleum and refinery engineering software

CL 611	Advanced Process Control	(3-0-0-6)
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Prerequisite: CL 309 or equivalent

Course contents:

Discrete time systems, analog to digital and digital to analog conversion, sampling of continuous time signal, conversion of discrete time to continuous time signal with zero and first order holds, z-transform, stability analysis of discrete time systems, Design of digital controller, Digital PID controller, Dahlin's algorithm, deadbeat controller, pole-placement and ringing. State-space representation of systems, discretization of state space model, transfer function to state space and state space to transfer function models, stability analysis of state space models, Lyapunov stability criteria, controllability and observability canonical forms, state observers, design of state space model based controller, model predictive controller, internal model controller.

Texts/References:

1. G. Stephanopoulos, Chemical Process Control: An Introduction to Theory and Practice, Prentice-Hall India, 2003.
2. W.L. Luyben, Process Modelling Simulation and Control for Chemical Engineers, McGraw-Hill, 1990.
3. B. Oggunnaik and W. H. Ray, Process Dynamics, Modeling and Control, Oxford University Press, 1995.
4. K. Ogata, Modern Control Engineering, Prentice Hall of India, New Delhi, 2003
5. B.W. Bequette, Process Control: Modelling Design and Simulation, Prentice Hall of India, New Delhi, 2003
6. K. Astrom and B. Wittenmark, Computer controlled Systems: System and Design, Prentice Hall of India, New Delhi, 1994
7. D.E. Seborg, T.F. Edgar and D.A. Mellichamp, Process Dynamics and Control, John Wiley & Sons Inc., 2003
8. W.L. Luyben, Process Modelling Simulation and Control for Chemical Engineers, McGraw-Hill, 1990.

CL 612	Colloid and Interface Science	(3-0-0-6)
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Course contents:

Basic concepts of colloids and interfaces; properties of colloidal dispersions; surfactants and their properties; micelles, bilayers, vesicles and liquid crystals; surface and interfacial tension; Young–Laplace equation; Kelvin equation; contact angle; intermolecular and surface forces; DLVO theory; adsorption at interfaces; characterization of solid surfaces; applications in detergents, personal-care products, pharmaceuticals, nanotechnology, and food, textile, paint and petroleum industries.

Texts/References:

1. P. C. Hiemenz and R. Rajagopalan, Principles of Colloid and Surface Chemistry, Marcel Dekker, New York, 1997.
2. J. C. Berg, An Introduction to Interfaces and Colloids: The Bridge to Nanoscience, World Scientific, Singapore, 2010.
3. P. Ghosh, Colloid and Interface Science, PHI Learning, New Delhi, 2009.
4. A. W. Adamson and A. P. Gast, Physical Chemistry of Surfaces, John Wiley & Sons, New York, 1997.
5. J. Israelachvili, Intermolecular and Surface Forces, Academic Press, New York, 1992.
6. R. J. Hunter, Foundations of Colloid Science, Oxford University Press, New York, 2005.

CL 613	Computational Fluid Dynamics	(3-0-0-6)
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Preamble:

Computational fluid dynamics (CFD) is an important tool for the analysis of chemical, petroleum and petrochemical processes. Analogical treatment is usually adopted for momentum, heat and mass transfer. The subject involves the application of numerical methods to solve problems associated to fluid flow in various machinery in the process industry. Such an approach is usually adopted to obtain a good understanding of the transport processes that are prevalent in various complex situations and thereby identify possible ways for enhancing the performance of the process. The course outlines various specific numerical methods that have been developed for the CFD. These are namely finite element method, finite volume method, finite difference method and boundary element methods. Further, the course also provides an introduction into turbulence modelling which enables furthering the application of CFD to vortices and eddies. The revised curriculum is broad to reflect upon the systematic learning of the student.

Course contents:

Introduction: Transport equations, Analytical and numerical solution of transport equations, Review of linear solvers; Analogical behaviour of momentum, mass and energy transport; Partial differential equations: types, boundary conditions; Finite difference, finite element and finite volume schemes: Grid generation and discretization; accuracy, consistency, stability and convergence; explicit and implicit formulation; solution of Navier-Stokes equation with various approach of simulation, staggered grid and collocated grid solution, Solution of Convective-diffusion equation; Solution of chemical engineering problems; Introduction to multiphase and turbulence modelling.

Texts/References:

1. S. V. Patankar, Numerical heat transfer and fluid flow, Taylor and Francis, 2004.
2. T. J. Chung, Computational Fluid Dynamics, Cambridge University Press, 2003.
3. P. S. Ghosdastidar, Computer simulation of flow and heat transfer, Tata McGraw Hill, 1998.
4. W. E. Schiesser and C. A. Silebi, Computational Transport Phenomena, Cambridge University Press, 1997.
5. S. K. Gupta, Numerical methods for engineers, New Age Intl., 2001.

CL 614	Fluidization Engineering	(3-0-0-6)
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Course content:

The phenomenon of fluidization; Liquid like behaviour of fluidized bed; Advantages and Industrial applications of fluidized beds; Dense bed fluidization; Distributors, gas jets and pumping power; Bubbles in dense beds; Bubbling fluidized beds; Entrainment and elutriation from fluidized beds; High velocity fluidization; Solid movement, mixing, segregation and staging; Gas dispersion and gas interchange in bubbling beds; mass and heat transfer between particle and gas; Heat transfer between fluidized beds and surfaces; Design of fluidized bed reactors.

Texts/References:

1. D. Kunii and O. Levenspiel, Fluidization Engineering, Butterworth, 1991.
2. D. Gidaspow, Multiphase Flow and Fluidization: Continuum and Kinetic Theory Description, Elsevier Science & Technology, 1993.
3. L.G. Gibilaro, Fluidization-dynamics, Butterworth-Heinemann, 2001.

CL 615	Optimization Techniques	(3-0-0-6)
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Preamble:

The existing curriculum in Optimization Techniques is exclusively towards evolutionary and stochastic programming techniques. Since many students don't have an in-depth understanding of non-linear optimization methods, the course first attempts to provide an elaborate syllabus content to conceptualize the need for evolutionary programming. The chosen topics include linear programming, non-linear programming, mixed integer non-linear programming etc. Eventually, the course provides a thorough understanding towards various evolutionary programming techniques including simulated annealing, genetic algorithm, particle swarm optimization, differential evolution etc. Eventually, various basic approaches adopted for the formulation of optimization models in process systems are summarized.

Course contents:

Optimization basics and convexity; Multi-dimensional constrained optimization: Gradient, Secant and Newton methods; Karsh-Kuhn-Tucker optimality conditions; Linear programming: Simplex method; Nonlinear programming: Sequential Quadratic Programming (SQP), generalized reduced gradient method (GRG) and penalty function methods; mixed integer linear programming (MILP), mixed integer nonlinear programming (MINLP), evolutionary optimization techniques: Genetic Algorithm, Simulated Annealing, particle swarm optimization, differential evolution, self-organizing migrating algorithm and scatter search; formulation of optimization models in process systems.

Texts/References:

1. G.V. Reklatis, A. Ravindran and K.M. Ragsdell, Engineering Optimization – Methods
2. S. S. Rao, Engineering Optimization: Theory and Practice, 4th Edition, John Wiley & Sons, 2009.
3. G. C. Onwubolu, Emerging Optimization Techniques in Production Planning and Control, Imperial College Press, 2002.
4. T. F. Edgar, D. M. Himmelblau and L. S. Lasdon, Optimization of Chemical Processes, McGraw - Hill, 2001.
5. L.T. Biegler, I.E. Grossmann and A.W. Westerberg, Systematic Methods of Chemical Process Design, Prentice Hall International Series, 1997.

CL 617	Petrochemicals	(3-0-0-6)
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Preamble:

The course on hydrocarbon processing exclusively deals with the production of petrochemicals from C1 to C4 hydrocarbons and hence, the course has been renamed as "Petrochemicals" from the existing "Petroleum Downstream Processing". Further, benzene, toluene and xylene (BTX) production has been included in the syllabus as these are the most valuable petrochemicals in the existing petrochemicals marketing sector and more than 100 chemicals are synthesized from these products. Similarly, polyethylene is also another important petrochemical product. Therefore, these topics have been added in the revised curriculum.

Course contents:

Petrochemical feedstock; Manufacture of acetic anhydride, acetone, acetic acid, adipic acid and aniline; Manufacture of benzene, toluene and xylene (BTX); Manufacture of benzoic acid, benzyl chloride, butyl acetate, carbon tetrachloride, chlorobenzene, ethyl acetate, maleic anhydride, methyl ethyl ketone, phthalic anhydride, polyvinyl chloride, polyethylene, propylene and vinyl acetate; Transportation of petrochemical products; Health and safety in petrochemical industries.

Texts/References:

1. M. Wells, Handbook of Petrochemicals and Processes, 2nd Ed., Ashgate Publishing Co., 1999.
2. S. Matar, Chemistry of Petrochemical Processes, 2nd Ed., Gulf Publishing Company, 2000.
3. P. Wiseman, Petrochemicals, John Wiley & Sons, 1986.
4. R. Meyers, Handbook of Petrochemicals Production Processes, McGraw Hill, 2005.

CL 618	Natural Gas Engineering	(3-0-0-6)
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Preamble:

The field of natural gas engineering is very much important for petroleum engineers specializing in gas processing technology. The course outlines an optimal balance between natural gas production, natural gas processing and gas transportation. While the core course CL 511 Petroleum Reservoir Engineering outlines the basic fundamentals in gas engineering, this course provides an extensive treatise on natural gas engineering involving both upstream and gas refining processes. The revised curriculum is carefully chosen to provide additional information to that presented in the reservoir engineering core course of the PST curriculum and eliminate the course content that is covered in the reservoir-engineering course.

Course contents:

Determination of natural gas properties such as specific gravity, pseudocritical properties, viscosity, compressibility factor, gas density, formation and expansion volume, and compressibility; Gas reservoir deliverability: analytical and empirical methods, construction of IPR curve, Well bore performance for both single and mist gas wells; Choke performance: Dry and wet gas flow in chokes; Well deliverability using nodal analysis; Natural gas processing: dehydration, gas treating, gas to liquids processing, compression and cooling; Natural gas transportation and measurement; advanced natural gas production engineering: Liquid loading, hydrate cleaning and pipeline cleaning.

Texts/References:

1. B. Guo and A. Ghalambor, Natural Gas Engineering Handbook, Gulf Publishing Company, 2005.
2. D.L. Katz and R.L. Lee, Natural Gas Engineering, McGraw-Hill, 1990.
3. B. Guo, W.C. Lyons and A. Ghalambor, Petroleum Production Engineering: A Computer Assisted Approach, Elsevier, 2007.
4. T. Ahmed and P. D. McKinney, Advanced Reservoir Engineering, Elsevier, 2005.

CL 619	Refinery Process Design [Revised]	(3-0-0-6)
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Preamble:

The revised syllabus thoroughly enables the student to relate upon his/her skill in chemical process design with the elements of refinery process design. The necessity to master graphical correlations is first thoroughly emphasized, as these correlations are required for the design and analysis of petroleum refinery processes. Eventually, refinery mass balances have been presented to extend the graphical concepts to design issues. Thereby, the course gradually trains the students to systematically learn the complexities associated in refinery design. For this purpose, first, light end units design procedures using Fenske-Underwood-Gilliland method are presented. Then, the design of multi-component refinery absorbers and strippers is presented using Kremser equations. Eventually, the most complicated design involving the design of Crude and Vacuum distillation units using extensively energy balances is presented. Finally, the design of refinery heat exchanger networks, FCC units and furnaces is addressed. This way, the revised syllabus adopts a systematic evolution of student's knowledge in the refinery process design.

Course contents:

Analogies between refinery and Chemical Process Design; Graphical and analytical correlations for refinery stream property estimation; refinery mass balances; design of oil-water separators; design of light end units using Fenske Underwood and Gilliland method; design of refinery absorbers and strippers; design of crude and vacuum distillation units; design of refinery heat exchanger networks; design of FCC units; furnace design.

Texts/References:

1. D. S. D. Jones, Elements of Petroleum Processing, John Wiley & Sons Inc., 1999
2. R. Smith, Chemical Process Design and Integration, John Wiley, 2005.
3. G.L. Kaes, Refinery process modeling, Elliott & Fitzpatrick Publishers, 2000.
4. R.E. Maples, Petroleum Refinery Process Economics, 2nd Ed., Pennwell Books, 2000.

CL 620	Nonlinear Bifurcation Analysis	(3-0-0-6)
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Preamble:

For general prospective, the title of the course has been renamed as "Nonlinear Bifurcation Analysis" from "CL 620 Nonlinear Analysis in Chemical Engineering". Nonlinear bifurcation analysis of a dynamical system is used to understand how solutions and their stability changes as the parameters in the system vary. In particular, it can be used for the computation, stability analysis and continuation of equilibria (steady-state solutions), and periodic and quasi-periodic oscillations. Steady state and dynamic behaviour of a standalone reactor and coupled with a separator for the first order elementary reaction and complex reactions are dealt with. This course will be beneficial for the students to find out the nonlinear behaviour of chemical process systems.

Course contents:

Introduction to mathematical modelling and bifurcation analysis; Bifurcation analysis of one dimensional dynamical system; Bifurcation analysis of higher dimensional dynamical systems: two dimensional system, three dimensional system; Bifurcation analysis of infinite dimensional system; Applications of bifurcation theory in chemical kinetics and engineering.

Texts:

1. R. Seydel, Practical Bifurcation and Stability Analysis, 3rd Ed., Springer, 2009.
2. S. Elnashaie, F. Uhlig and C. Affane, Numerical Techniques for Chemical and Biological Engineers using MATLAB, Springer, 2007.
3. S. Pushpavanam, Mathematical Methods in Chemical Engineering, Prentice Hall of India, 2001.

References:

1. P. M. Gray and S. K. Scott, Chemical Oscillation and Instabilities: Nonlinear Chemical Kinetics, Oxford University Press, 1990.
2. R. Aris, Elementary Chemical Reactor Analysis, Courier Dover Publications, 1999.
3. I. R. Epstein and J. A. Pojman, An Introduction to Nonlinear Chemical Dynamics Oscillations, Waves, Patterns, and Chaos, Oxford University Press, 1998.

CL 622

Molecular Simulations: Principles and Applications

(3-0-0-6)

Course contents:

Fundamentals of molecular simulations–Ab-initio methods, basis sets, Hartree-Fock theory, density functional theory, geometry optimization, vibrational analysis; elementary, classical statistical mechanics, elementary concepts of temperature, ensembles and fluctuations, partition function, ensemble averaging, ergodicity; molecular dynamics methodology – force field, integral ng algorithms, periodic box and minimum image convention, long range forces, non-bonded interactions, temperature control, pressure control, estimation of pure component properties, radial distribution function; molecular dynamics packages; Monte Carlo simulation –Monte Carlo integration, simple biasing methods, importance sampling, Markov chain, transition-probability matrix, detailed balance, Metropolis algorithm; Monte Carlo simulation in different ensembles; Monte Carlo simulation for polymer; advanced topics.

Texts/References:

1. D. Frenkel and B. Smit, Understanding Molecular Simulation: From Algorithms to Applications, 2nd Ed., Academic Press, New York, 2002.
2. M.P. Allen and D.J. Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford, 1987.
3. D. A. McQuarrie, Quantum Chemistry. Viva Books, New Delhi, 2003
4. K. Binder, The Monte-Carlo Method in Condensed Matter Physics, Springer-verlag, Berlin,1992.
5. M. H. Kalos and P. A. Whitlock, Monte Carlo Methods, Vol. I, Basics, Wiley, New York,1986
6. D. A. McQuarrie, Statistical Mechanics, Harper and Row, New York, 1976.
7. A. R. Leach, Molecular modelling: principles and applications, 2nd Ed., Pearson Education, New Delhi, 2001

CL 623	Polymer Science and Technology	(3-0-0-6)
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Course contents:

Classification of polymers; polymer structure; molecular weight; chemical structure and thermal transition; synthesis of polymers; polymerization mechanism and techniques; phase behaviour, thermodynamics and molecular weight determination; solid state properties of polymers; viscoelasticity and rubber elasticity; degradation, stability and environmental issues; polymer additives, blends, composites, thermoplastics, fibres, elastomers, thermosets, and specialty polymers; polymer processing, rheology and analysis using non-Newtonian fluid model; applications of polymers in separations

Texts/References:

1. P. J. Flory, Principles of polymer chemistry, Asian Books, 2006
2. M. Rubinstein and R. H. Colby, Polymer physics, Oxford University Press, USA, 2003
3. N. K. Petchers, R. K. Gupta, and A. Kumar, Fundamentals of Polymer Engineering, 2nd Ed., Marcel Dekker, 2003.
4. J. R. Fried, Polymer Science & Technology, Prentice Hall of India, 2nd Ed., 2009.
5. F. W. Billmeyer (Jr.), Text Book of Polymer Science, 3rd Ed., John Wiley & Sons, 2002.
6. P. Bahadur and N. V. Sastry, Principles of Polymer Science, Narosa Publishing House, 2002
7. V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, Polymer science, New Age International (P) Ltd., 2001

CL 624	Computing in Chemical and Petroleum Engineering	(2-0-2-6)
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Preamble:

The course "CL 624 Computing in Refinery Engineering" is renamed as "Computing in Chemical and Petroleum Engineering" as a result of title change in M.Tech. Specialization from "Petroleum Refinery Engineering" to "Petroleum Science and Technology". Mathematical modelling and computer simulation in chemical and petroleum engineering is indispensable in design, optimization, and control of processes, and even the entire process plants. In this context, this course gives the state of the art information from the point of view of undergraduate and postgraduate students in chemical engineering and petroleum engineering, respectively. This is an integrated curriculum, which teaches the mathematical formulation of the problems from first principles, the computer programs needed to solve these problems, and how to ensure that the problems have been solved correctly. The course on computing in chemical and petroleum engineering covers the topics on chemical reaction engineering, process systems engineering, thermodynamics, transfer operations, petroleum reservoir engineering, petroleum refinery engineering, and so on. This course will be beneficial for the students to enhance his/her computational skills to solve the engineering problems.

Course contents:

Introduction to chemical engineering computing; Nonlinear parameter estimation; Computation of thermodynamic properties; Computation of vapour-liquid and chemical reaction equilibria; Transport processes: momentum, heat and mass transfer; Modelling of chemical processes; Lumping analysis in petroleum processing; computation of properties of petroleum fractions; Kinetic modelling in processing of heavy petroleum fractions; Applications of computing in chemical, petroleum reservoir, and refinery engineering.

The following modules are to be solved by using mathematical software in the laboratory sessions. Problem solving through computer aided numerical methods Fitting of vapour pressure data with the correlations Kinetic parameter estimation through hybrid particle swarm optimization Calculation of thermodynamic properties of pure components and crude oils using equations of state Computation of equilibrium constants in petroleum engineering Flash calculation in petroleum engineering Simulation of chemical process Lumping analysis in modelling of petroleum processes Computation of properties of petroleum fractions Simulation of refinery processes

Texts:

1. B. A. Finlayson, Introduction to Chemical Engineering Computing, Wiley publication 2006.
2. M. B. Cutlip, Mordechai Shacham, Problem Solving in Chemical and Biochemical Engineering with POLYMATH, Excel, and MATLAB, Prentice Hall, 2008.
3. M. A. Fahim, T. A. Al-sahhaf and A. Elkilani, Fundamentals of Petroleum Refining, Elsevier Science & Technology, 2010.
4. A. Tarek, Working Guide to Vapor-Liquid Phase Equilibria Calculations, Gulf Professional Publishing, 2010.

References:

1. B. E. Poling, J. M. Prausnitz and J. P. O'Connell, The Properties of Gases and Liquids, 5th Ed., McGraw Hill, 2001.
2. L. T. Biegler, A. W. Westerberg and I. E. Grossmann, Systematic Methods of Chemical Process Design, Prentice Hall, 1997.
3. R. Smith, Chemical Process Design and Integration, 8th Ed., Wiley-India, 2006.
4. S. Skogestad, Chemical and Energy Process Engineering, CRC press, 2009.
5. S. C. Chapra, Raymond P. Canale, Numerical Methods for Engineers, 6th Ed., McGraw Hill, 2010.
6. A. Tarek, Reservoir Engineering Handbook, 4th Ed., Gulf Professional Publishing, 2010.
7. G. L. Kaes, Refinery Process Modeling, Kaes Enterprises, 2000.
8. R. A. Meyers, Handbook of Petroleum Refining Processes, 3rd Ed., McGraw Hill, 2003.

CL 625

Fundamentals of Micro-Nano Fluidics and Micro-Fabrication

(3-0-0-6)

Course contents:

Principles of Mesoscale heat, mass and momentum transport; Fundamentals of vector/tensor algebra/calculus and order of magnitude analysis; Stability analysis: linear, weakly-nonlinear, and nonlinear; Instabilities: Rayleigh-Benard, Rayleigh-Taylor, Kelvin- Helmholtz, and Saffman-Taylor; Thin film dynamics and colloidal domain; Intermolecular and capillary forces; Electro- hydrodynamics (EHD): Maxwell stresses; electro-kinetics, zeta- potential; Magneto-hydrodynamics (MHD); Micro-nano fabrication: photolithography; Principles of Microscopes; Principles of spectroscopic studies; Fundamentals of chromatography; Fabrication and characterization in mesoscale employing lithography, microscopy, chromatography and spectroscopy.

Texts/References:

1. L. G. Leal, Advanced Transport Phenomena Fluid Mechanics and Convective Transport Processes, 1st Ed., Cambridge Series in Chemical Engineering, 2007.
2. M. J. Madou, Fundamentals of Microfabrication: The Science of Miniaturization, 2nd Ed., Taylor & Francis, Inc., 2002.
3. S. Chakraborty, Microfluidics and Microfabrication, 1st Ed., Springer, 2010.

CL 626	Energy Resources	(3-0-0-6)
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Preamble:

Energy is vital to all our endeavours and, indeed, to the maintenance of life itself. Energy exists in many forms such as chemical energy, nuclear energy, solar energy, mechanical energy, electrical energy, internal energy in a body, bio-energy in vegetables and animal bodies, thermal energy etc. We also observe the various activities around us are 'energy transformations'. The objective of this course is to provide a comprehensive coverage of energy resources and conversion.

Course contents:

Introduction, major sources of energy: renewable and non-renewable, primary and secondary energy sources, energy scenario, prospects/need of alternate energy sources, conventional and non-conventional energy sources; solar energy; wind energy; nuclear energy; geo-thermal, hydro energy sources; tidal energy; energy from biomass; energy from coal; and other energy resources: hydrogen, fuel cells; environmental aspects of energy utilization-renewable energy resources and their importance; combustion process: combustion stoichiometry and combustion thermodynamics; gas burners; oil burners; coal burning equipment; Integrated energy system: concept of integration of conventional and non-conventional energy resources and systems; energy conservation & management.

Texts/References:

1. S. Sarkar, Fuel & combustion, Orient Longman, 2nd Ed., 1990.
2. J. G. Speight, Fuel Science & Technology Handbook, Dekker, 1990.
3. R. E. Haytes, and S.T. Kocackowski, Introduction to catalytic combustion, Gordon Beach, 1997.
4. B. H. Khan, Non-conventional energy resources, McGraw Hill, New Delhi.
5. C. S. Solanki, Renewable energy Technology, Prentice Hall Publication, 2008.
6. S. P. Sukhatme, Solar Energy, Tata McGraw Hill, New Delhi, 1996.
7. W. C. Turner, Energy management handbook, Wiley Press, 1982.

CL 627

Multiphase Flow

(3-0-0-6)

Preamble:

Multiphase flow reactors are critically important in industrial applications across many sectors of the economy. Conventional industries as varied as petroleum refining, petrochemicals, bulk and fine chemicals, mineral processing, pharmaceuticals, energy and power, paper manufacturing, food processing, as well as the "new economy" industries such as bio-medical, nanotechnology, micro-electro-mechanical systems (MEMS), micro-total analysis systems (μ TAS), all have multiphase reactors and contactors at the heart of their respective processes. Further, multiphase flow is an important topic in the field of petroleum engineering discipline. Therefore, it is important to teach the behaviour of multiphase flow vessels at 'Masters' level. In this course, behaviour of different type of multiphase flows (gas-liquid, gas-solids, liquid-solids and gas-liquid-solids) will be taught at different scales starting from macro-scale to micro-scale. Further, different advanced modelling tools and measurement techniques will be discussed.

Course contents:

General scope and features of multiphase flows; Fundamental definitions and terminology; Flow Pattern of multiphase flows: flow-pattern map for fluid-fluid, fluid-solid and three phase flows; Pressure drop and void fraction; Multiphase interactions: interactions of fluids with particles, drops and bubbles; Multiphase flow through porous media; Micro-scale flows: introduction to gas-liquid two-phase flow in micro-channels, two-phase flow patterns in micro channels; Overview of multiphase flow modelling; Multiphase flow measurements: Invasive and non-invasive.

Texts/References:

1. G. Wallis, One Dimensional Two Phase Flows, Mc-Graw Hill, 1969.
2. C. E. Brennen, Fundamentals of multiphase flow, Cambridge University Press, 2005.
3. C.T. Crowe, Multiphase Flow Handbook, CRC Press, 2005.
4. N.I. Kolev, Multiphase Flow Dynamics 1: Fundamentals, Springer, 2007.
5. C.M. Marle, Multiphase Flow in Porous Media, Technip, 1981.

CL 628	Catalysts and Adsorbents	(3-0-0-6)
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Preamble:

Catalysts and adsorbents are integral part of chemical industries, which are associated with all major sectors of world economy. Therefore, it is essential for chemical engineers to have comprehensive knowledge about catalyst and adsorbent materials. This course teaches the basic theories of catalysis and adsorption along with types, preparation, physicochemical properties and application of the materials in details. This course also acquaints the students with latest developments in catalyst and adsorbent materials in different sectors.

Course contents:

Fundamentals of catalysis and adsorption; types of catalysts and adsorbents, preparation methods: conventional and novel; surface area and porosity; bulk and surface characterizations, diffusion in porous material, kinetics and mechanisms; transport effect; deactivation; major applications; recent developments in catalysts and adsorbents.

Texts/References:

1. J. M. Smith, Chemical Engineering Kinetics, McGraw-Hill Book Company, 1981
2. D. M. Ruthven, Principles of adsorption and adsorption processes, John Wiley & Sons, 1984.
3. R.T. Yang, Adsorbents: Fundamentals and Applications, Wiley-Interscience, 2003.
4. K.P. de Jong, Synthesis of solid catalysts, Wiley-VCH, 2009
5. H. S. Fogler, Elements of Chemical reaction engineering, Prentice Hall of India., 1999
6. C. H. Bartholomew and R. J. Farrauto, Fundamentals of Industrial catalytic Processes, Wiley-VCH, 2006
7. J. M. Thomas and W. J. Thomas, Principles and Practice of Heterogeneous Catalysis, Wiley-VCH, 1996
8. R.T. Yang, Gas Separation By Adsorption Processes, World Scientific Publishing Company, 1997 G. Ertl, H. Knozinger and J. Weitkamp, Handbook of Heterogeneous Catalysis, Vols. 1-2, Wiley- VCH, 1997

CL 629	Membranes	(3-0-0-6)
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Preamble:

Membranes are becoming the most important, practically useful and popular materials for applications to modern separation technique in chemical, biochemical, food, petrochemical and several allied process industries. Some of the membrane based separation processes have attained considerable maturity to successfully compete with the traditional separation processes due to the advantages like: low energy consumption, easy scale-up, non-requirement of any additives or usefulness as a part of hybrid processes. Membranes are manufactured from different materials like polymeric, ceramic, zeolite and can be accommodated in different kind of modules like tubular, spiral, capillary, plate - and- frame, and hollow fibre. However, syntheses of target specific and highly selective membranes with narrow pore size distribution are some of the present day challenges. Concentration polarization and fouling are also the biggest problems of membrane processes. The present course aims at familiarizing the students with the various methods of synthesis of different kinds of membrane along with their characterization procedures and applications. They will also be acquainted with the latest developments of new membrane materials and processes.

Course contents:

Introduction to membranes; membrane materials: polymeric, inorganic and liquid; membrane preparation: phase inversion, immersion precipitation, track-etch method, sol- gel process, interfacial polymerization, dip-coating process, film stretching and template leaching; characterization of membranes; transport in membranes; various membrane processes and applications; concentration polarization and fouling; membrane modules and process design; membrane reactors and membrane bioreactors.

Texts/References:

1. M. H. Mulder, Basic Principles of Membrane Technology, Springer, 2004.
2. B. K. Dutta, Mass Transfer and Separation Processes, PHI, 2007.
3. M. Cheryan, Ultrafiltration & Microfiltration Handbook, Technomic, 1998.
4. K. Nath, Membrane Separation Processes, PHI, 2008.

CL 630	Composite Materials	(3-0-0-6)
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Preamble:

Composites science and technology is an emerging area of materials science because certain inherent advantages of composites. Aircraft and spacecraft are typical weight sensitive structures in which composite materials are cost effective. Polymer-clay nanocomposite is one of the thrust areas of research in the field of composites. Thus, a course on composite materials is highly relevant in the curriculum while studying materials science and technology. The objective of this course is to provide the basic concepts of composite materials. This course involves manufacturing processes, anisotropic elasticity, strength of anisotropic materials, etc. A comprehensive introduction to composite materials and motivation for their use in current structural applications is covered in detail. Stress-strain relations for a lamina are demonstrated with engineering material constants, too. Lamination theory is presented with the aid of new laminate classification scheme. Moreover, the subject will reveal a high level of comparison between theory and experimental results in order to create the confidence in the derived theory.

Course contents:

Definition of composites; classification; particulate filled and fibre reinforced composites; ceramic composites, resin based composites, composite semiconductors, polymer-metal composites; polymer nanocomposites; theory of reinforcement; concept of microfibril; effect of orientation and adhesion; composite properties; lamination theory; mechanical behaviour of composites: stress - strain relationship, strength, fracture, toughness and fatigue; composites fabrication.

Texts/References:

1. R.M. Jones, Mechanics of Composite Materials, Second Edition, 1st Indian Reprint, Taylor & Francis, 2010.
2. F. L. Matthews and R. D. Rawlings, Composite Materials: Engineering and Science, CRC Press, Woodhead, 1999.
3. B.D. Agarwal, and J.D. Broutman, Analysis and Performance of Fiber Composites, John Wiley and Sons, New York, 1990.
4. P.K. Mallik, Fiber reinforced composites: materials, manufacturing and design, 2nd Ed., Marcel and Dekker, New York, 1993.
5. K.K. Arthur, Mechanics of Composite Materials, CRC Press, 1997.
6. P.K. Mallik, Composite Engineering Hand Book, 2nd Ed., Marcel and Dekker, New York, 1997.

CL 631	Smart Materials	(3-0-0-6)
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[An elective Course for M.Tech. (Specialization: Materials Science & Technology)]

Preamble:

The objective of this course is to develop the knowledge and awareness of smart materials and concepts to engineering application areas. Students will acquire a critical understanding of mechanisms giving rise to the characteristic and beneficial properties of smart materials. The recent state-of-art on the technological applicability and limits of smart materials will be discussed. The course will provide a basis of understanding for many of the materials and material systems that underlie the analysis and design of "smart" devices.

Course contents:

Introduction to smart materials: definition, type, properties and examples; Modelling of mechanical and electrical system: fundamental relationships in mechanics and electrostatics, work and energy; Mathematical representations of smart material system: first order and second order dynamic systems, frequency response; Piezoelectric materials, shape-memory materials, conductive polymers, pH and temperature sensitive polymer; Engineering and scientific applications of different smart materials, their preparation, characterization and use as smart products; Smart membrane, smart healable materials and chromogenic smart material; Biologically and field responsive smart materials; Applications of different smart materials.

Texts/References:

1. D. J. Leo, Engineering Analysis of Smart Materials Systems, Wiley, 2007.
2. M.V. Ghandi and B.S. Thompson, Smart Materials and Structures, Chapman & Hall, 1992.
3. A.V. Srinivasan and D.M. McFarland, Smart Structures, Cambridge University Press, 2001.
4. H. Janocha (Ed.), Adaptronics and Smart Structures, Springer, 1999.
5. R.C. Smith, Smart Material Systems: Model Development (Frontiers in Applied Mathematics), SIAM, 2005.

CL 632

Integration of Refinery and Petrochemical Operations

(2-0-2-6)

[Departmental Elective for M. Tech (Petroleum Science & Technology (PST))]

Preamble:

For decades, refineries and petrochemical industries have enjoyed an enviable position of being able to dominate their respective market, as there were very few competitive alternatives. However, both these industries are being increasingly plagued by a number of factors including geo-political tensions, continuous depletion of oil resources and increasing competition from other alternatives. In addition to enhancing the energy security of the nation, many of these alternatives are renewable and possess a smaller carbon footprint that has contributed to their wide acceptance in the society. Under these challenging circumstances, the viability and long-term sustainability of both the refinery and the petrochemical industry would depend on how well it uses its resources and continues to maintain its competitive edge over its alternatives. Many of these challenges can be addressed by harnessing the synergy between the refinery and petrochemical industry by a seamless integration. Such integration could prove beneficial to all stakeholders as it enables better utilization of the precious non-renewable resources, minimizes the investment risks and reduces the environmental impact. However due to their inherent complexities, the integration of refinery and petrochemical industries requires a rigorous mathematical approach and is an active area of research. The objective of this course is to provide a mathematical background to its participants and apprise them of the current practices thereby enabling them to contribute to this growing and exciting area of research. The course would also familiarize the participants with some of the state- of-the-art modelling and optimization packages.

Course Contents:

Synergy between Overview of Petroleum Refining and Petrochemical Industries; Refinery and Petrochemical Industry; Process and Utility Integration; Introduction to Optimization Techniques and Sensitivity Analysis; Deterministic Planning and Planning under Uncertainty Multisite Refinery Network Integration, Multisite Refinery and Petrochemical Network Integration; Cost Estimation and Economic Evaluation; Computer aided solution of integration models.

Texts/References:

1. K.Y. Al-Qahtani and A. Elkamel, Planning and Integration of Refinery and Petrochemical Operations, Wiley- VCH, 2010.
2. J.H. Gary, G. E. Handwerk and M. J. Kaiser, Petroleum Refining: Technology and Economics, 5th Edn., CRC Press, 2007.
3. T. Edgar, D. Himmelblau and L. Lasdon, Optimization of Chemical Processes, 2nd Edn., Tata McGraw Hill, 2001.
4. G. C. Onwubolu, Emerging Optimization Techniques in Production Planning and Control, Imperial College Press, 2002.
5. R. M. Smith, Chemical Process: Design and Integration, Wiley Publications, 2005.
6. R. Maples, Petroleum Refinery Process Economics, 2nd Edn., PennWell Books, 2000.

CL 633

Applied Statistical Thermodynamics

(3-0-0-6)

[Open Elective]

Preamble:

With the present emphasis on nano- and biotechnologies, molecular-level descriptions can be used to make useful predictions in the area of chemical engineering and physical chemistry. While classical thermodynamics can be used to interrelate heat and work; and describe many processes such as phase behaviour, chemical reaction equilibria, and flows on changes of state, it barely acknowledges the existence of molecules. Statistical thermodynamics, which starts with a description of individual molecules, can provide such information. Non-interacting molecules lead to an understanding of the ideal gas, where the road is an easier one. However, as it will be evident in the course that the analysis for molecules that interact (especially in a dense fluid such as a liquid) is more complicated, and generally cannot be solved exactly. Nonetheless, we can obtain useful insights by starting with a molecular-level description and statistical thermodynamics. In this course only equilibrium properties are considered here, not dynamic or kinetic properties like the kinetic theory of gases or liquids; hence the use here of the term statistical thermodynamics rather than the more general term statistical mechanics.

Course contents:

Introduction to Statistical Thermodynamics; Canonical Partition Function; Partition Function for Ideal, Monoatomic, Diatomic and Polyatomic Gases; Micro canonical Ensemble for a Pure Fluid; ; Grand Canonical Ensemble for a Pure Fluid Isobaric-Isothermal Ensemble ; Restricted Grand or Semi-Grand Canonical Ensemble ; Interacting Molecules in a Gas; Interaction Potential and Evaluation of Second Virial Coefficient ; Development of Equations of State from Lattice Theory; Activity Coefficient Models for Similar-Size Molecules from Lattice Theory; Interacting Molecules in a dense fluid; Integral Equation Theories for Radial Distribution Functions.

Texts and References:

1. S. I. Sandler, An Introduction to Applied Statistical Thermodynamics. John Wiley & Sons. Hoboken, NJ, 2010.
2. D. A. McQuarrie, Statistical Mechanics, University Science Books, Sausalito, CA, 2000.
3. D. Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press, London, 1987.
4. K. A. Dill and S. Bromberg, Statistical Thermodynamics in Chemistry and Biology, Garland Science, New York, 2003.
5. M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford, 1989
6. J. S. Rowlinson and F. L. Swinton, Liquids and Liquid Mixtures, 3rd ed., Butterworths, Oxford, 1982.

CL-634	Applied Rheology	(3-0-0-6)
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Preamble:

Non-Newtonian fluids are often used in our day-to-day life as well as in many chemical, biochemical, pharmaceutical, polymer industries, etc. Some of the daily-life applications include personal care products such as cosmetics, gels, pastes; food stuffs such as sandwich spreads, ketchup, chocolate, soups, etc. Some of the industrial applications include processing of many polymers, paints and detergents, degassing of polymeric melts and glasses, use of non-Newtonian polymers in enhanced oil recovery wherein oil droplets become suspended in non-Newtonian polymer solutions and/or during their transport in the form of oil-in-polymer solution emulsions, non-Newtonian fluidized beds, wastewater treatment, production of polymeric alloys and ceramics via liquid routes, pharmaceutical products wherein the polymer thickening agents are used to enhance their stability for extended shelf-life, pulp and paper industries, etc. Because of aforementioned overwhelming applications, it is required for both undergraduate and postgraduate students to acquire enough academic experience related to the momentum, heat and mass transfer phenomena associated with non-Newtonian fluids.

Prerequisite: Basic fluid mechanics and/or transport phenomena at UG level

Open for: Ph.D. (Chemical), M.Tech. (PST/MST) and 4th year B.Tech. (Chemical)

Course Contents

Basics of non-Newtonian fluid behaviour, classification of non-Newtonian fluids, rheometry such as sliding plates, falling ball, concentric cylinder, parallel disks and cone and plate rheometers for non-Newtonian fluids, pressure-driven non-Newtonian flows, free and hindered settling of particles in non-Newtonian suspensions, flow of non-Newtonian fluids in pipes, infinite parallel plates and concentric annulus, criteria for transition from laminar to turbulent flow of non-Newtonian fluids, miscellaneous frictional losses and selection of pumps for flow of non-Newtonian fluids, flow of multiphase mixtures in pipes, heat transfer characteristics of non-Newtonian fluids in pipes and between channels, momentum, heat and mass transfer in boundary layers flows of non-Newtonian fluids, and mixing of non-Newtonian fluids.

Texts/References

1. R.P. Chhabra and J.F. Richardson, Non-Newtonian Flow and Applied Rheology, 2nd Edition, Butterworth-Heinemann, Oxford, UK, 2008.
2. Christopher W. Macosko, Rheology: Principles, Measurements, and Applications, Wiley-VCH, New York, 1994.
3. R. Brummer, Rheology Essentials of Cosmetic and Food Emulsions, Springer, Heidelberg, Germany, 2006.
4. J.W. Goodwin and R.W. Hughes, Rheology for Chemists: An Introduction, 2nd Edition, RSC Publishing, Cambridge, UK, 2008.
5. M.A. Rao, Rheology of Fluid and Semisolid Foods: Principles and Applications, 2nd Edition, Springer, New York, 2007.

CL 635	Advanced Clean Fuel Technologies	(3-0-0-6)
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Preamble:

The aim of the course is to provide the recent trends in processing and utilization of fossil fuel as a clean source. First part of the course teaches the conventional and advanced technologies of combustion and gasification. Secondly, it covers the gas cleaning and advanced power generation technologies concerning the efficient utilization of the clean fuel. Finally, the course elaborates the existing advanced clean coal technologies mainly for carbon capture and storage. In overall, the syllabus covers complete representation of the conventional and advanced clean fuel technologies.

Course Contents:

Combustion and gasification technologies: Introduction, Fuel characteristics, Energy and exergy analysis, Process parameters, Conventional fixed, fluidized and entrained bed combustion and gasification, Biomass combustion and gasification, Co-combustion, Oxy- fuel combustion and flame moderation, Chemical looping combustion, High temperature air combustion, Supercritical and ultra-supercritical boilers, NO_x and SO_x emission control burners; Gas cleaning technologies: H₂S, COS, NO_x, SO_x removal, Hot gas cleaning; Power generation technologies: Gas turbines, Steam turbines, Integrated gasification combined cycle (IGCC), Fuel based hybrid power generation; Clean coal technologies: Underground coal gasification, Coal bed methane, Coal beneficiation, CO₂ enhanced oil recovery, CO₂ sequestration, Coal to hydrogen and liquid fuels.

Texts and References:

1. S. R. Turns, An Introduction to Combustion, 3rd Ed., McGraw Hill, 2012.
2. I. Glassman, R. A. Yetter, Combustion, 4th Ed., Academic Press, 2009.
3. A. Williams, M. Pourkashanian, N. Skorupska, J. M. Jones, Combustion and Gasification of coal, Taylor and Francis, 2000.
4. J. G. Speight, The Chemistry and Technology of coal, 2nd Ed., Dekker, 1994.
5. P Breeze, Power generation technologies, Newnes, 2005.
6. L Zheng, Oxy-fuel combustion for power generation and carbon dioxide (CO₂) capture, Woodhead Publishing Series, 2011.

CL 636	Microelectronic Fabrication	(3-0-0-6)
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Preamble:

The course Microelectronic Fabrication as indicated below, has been proposed with emphasis on key processes in the chip manufacturing. This course will provide the fundamental concepts of various processes involved in chip manufacturing such as photolithography, deposition and material removal. In addition, the MOS structure and operation will also be given to understand the sequence of processes used in creating transistor. The topics such as process integration, testing and yield, which are relevant for the industry, would also be covered.

Course Contents:

Introduction: Review of Chip Manufacturing Process, FEOL and BEOL concepts; Photolithography: Lithography basics, Wavelength, Layout and Optical Proximity Correction (OPC), Mask making, Phase shift mask, Lithography details, Production issues including depth of focus, misalignment; Deposition: Physical and Chemical Vapour Deposition (PVD & CVD) basics, Electrochemical deposition; Material Removal: Plasma and wet etching, Chemical Mechanical Polishing (CMP) basics, Dishing, Erosion, Issues in Shallow Trench Isolation, Oxide Polish and Copper Polish, Post CMP issues; FEOL: Semiconductor electron band structure, band gap MOS capacitor, MOS transistor structure for enhancement mode devices, Transistor fabrication, MOS transistor operation; Diffusion and Ion implantation: Implantation basics, Constant source and limited source diffusion, Diffusion vs. ion implantation, Mechanism and Models, Equipment, relevant issues; Oxidation: Process Types, Details of thermal oxidation, Models, relevant issues; Process Integration: BEOL Issues, Cu vs. Al metallization, oxide vs. low-k integration, MEMS; Testing and Yield: Scribe line Test (for process evaluation), Functional Test (for product evaluation), Yield Models, process and design modifications for yield optimization.

Texts and References:

1. S.A. Campbell, The Science and Engineering of Microelectronic Fabrication, 2nd Edition, Oxford University Press, 2001
2. Richard C. Jaeger, Introduction to Microelectronic Fabrication, Vol. 5 of Modular Series on Solid State Devices, 2nd Edition, Prentice Hall, 2001
3. C.Y. Chang and S.M. Sze, ULSI Technology, McGraw Hill, 1996
4. Peter Van Zant, Carol Rose (Editor), Daniel Gonneau (Editor), Microchip Fabrication: A Practical Guide to Semiconductor Processing, 2nd Edition, Semiconductor devices, 1990.

CL 637

Multicomponent Mass Transfer (MMT)

(3-0-0-6)

Preambles:

This course deals with the basic equations of diffusion in multicomponent systems to provide a sound background in the fundamentals of multicomponent mass transfer. Understanding the origins of various mass transfer models and its relationship to the equations governing conservation of mass, momentum, and energy for the simulation and design of process equipment, will be addressed. An exposure to simplified models for mass transfer in laminar and turbulent flows, along with algorithms to implement such models in software tools such as Matlab, Polymath, etc. will be provided.

Course Contents:

Flux Concepts, Reference Frames, Diffusion in Multicomponent Systems, Maxwell-Stefan Relations, Generalized Fick's Law for Multicomponent Systems, Estimation of Diffusion Coefficient, Linearized Theory, Effective Diffusivity Models, Interphase Mass Transfer, BL Theory, Penetration Theory, Introduction to Turbulence, Simultaneous Mass and Energy Transfer, Applications of Multicomponent Mass Transfer Models for Simulation and Design of Process Equipment.

Texts and References:

1. R. Taylor and R. Krishna, Multicomponent Mass Transfer, John Wiley & Sons Inc. Edition 1st, 1993.
2. J. A. Wesselingh and R. Krishna, Mass Transfer in Multicomponent Mixtures, Delft Academic Press. Edition 1st, 2000.
3. R. B. Bird, W.E. Stewart, and E.N. Lightfoot, Transport Phenomena, John Wiley and Sons. Edition 2nd, 2006.
4. A. L. Hines, R. N. Maddox, Mass Transfer, Prentice-Hall, Inc. Edition 1st, 1985.
5. E. L. Cussler, Diffusion, Mass Transfer in Fluid Systems, Cambridge University Press. 2009, Edition 3rd.

CL 638	Mathematical Methods in Chemical Engineering	(3-0-0-6)
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Prerequisite:

- Transport Phenomena
- Chemical Reaction Engineering

Preamble:

The course CL 638: Mathematical Methods in Chemical Engineering (3-0- 0-6), as indicated below, has been proposed with emphasis on enhancing students' knowledge of calculus, linear algebra, and differential equations by applying appropriate examples and applications from chemical engineering. This course is designed to illustrate the techniques that chemical engineers need to know to effectively model, analyse, and carry out numerical simulations of various chemical engineering processes. This course deals with the development and application of mathematical methods for the solution of chemical engineering problems. Major emphasis is given to the mathematical implications of describing and solving representation of chemical engineering systems. Case studies relevant to ongoing research activities will be addressed.

Course Contents:

Application of Dependent/Independent Vectors, Orthogonal and Orthonormal Vectors, Gram-Schmidt Orthogonalization, Matrix and Determinants in Chemical Engineering Problems Ordinary Differential Equations and Adjoint Operators: Properties of Adjoint Operators; Theorem for Eigenvalues and Eigen functions; Applications of Eigenvalue Problems in Chemical Engineering Systems; Stability Analysis, Bifurcation Theory; Examples using Chemical Engineering Systems Solution of Partial Differential Equations; Laplace Transformation; Fourier Transformation; Applications to Problems from Fluid Mechanics, Heat Transfer and Mass Transfer Solution of Linear and Non-linear Algebraic Equations by Numerical Techniques: Applications to Problems from Fluid Mechanics, Heat Transfer and Mass Transfer

Texts and References:

1. S. Pushpavanam, Mathematical Methods in Chemical Engineering, Prentice Hall of India, 1998.
2. R. G. Rice and D. D. Do, Applied Mathematics and Modeling for Chemical Engineers, 2nd Ed., Wiley, 2012.
3. A. Varma and M. Morbidelli, Mathematical Method in Chemical Engineering, Oxford University Press, 1997.
4. N. W. Loney, Applied Mathematical Methods for Chemical Engineers, 2nd Ed., CRC Press, 2006.
5. V. G. Jenson and G. V. Jeffreys, Mathematical Methods in Chemical Engineering, 2nd Ed., Academic Press, 1978.
6. S. K. Gupta, Numerical Methods for Engineers, 3rd Ed., New Academic Science, 2013.
7. J. N. Reddy, An Introduction to the Finite Element Method, 3rd Ed., McGraw-Hill, 2005.

CL 639	Biofluid Mechanics	(3-0-0-6)
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Preamble:

With rapid advancements in the biomedical science and engineering, there is a need for engineers with knowledge in multiple disciplines. This course aims to develop an understanding of the role fluid dynamics plays in the human circulatory system among students from Chemical Engineering, Mechanical Engineering and Biotechnology background. The course is an introduction to the physiologically relevant fluid flow phenomena and underlying physical mechanisms from the viewpoint of an engineer.

Prerequisites: A course on basics fluid mechanics.

Syllabus:

Cardiovascular and pulmonary physiology, Rheology of blood, blood flow in small tubes and capillaries, blood flow in large arteries, air flow in the lungs and the mechanics of breathing, synovial fluid in joints, flow and pressure measurement techniques in human body, CFD analysis of human circulation.

Text and Reference Books:

1. Chandran, B. K., Rittgers, S. E. and Yoganathan, A. P. "Biofluid Mechanics", CRC Press, Second edition, 2012.
2. Waite, L., Fine, J. "Applied Biofluid Mechanics", McGraw Hill, 2007.
3. Pedley, T. J. "The fluid mechanics of large blood vessels", Cambridge University Press, 1980.
4. Mazumdar, J. N. "Biofluid Mechanics", World Scientific, Inc., 1992.
5. Guyton, A. C. and Hall, J. E. "A textbook of medical physiology", tenth edition, W. B. Saunders Company, Philadelphia.
6. Truskey, G. A., Yuan, F. and Katz, D. F. "Transport Phenomena in biological systems", 2nd edition, Prentice Hall, 2009.
7. Phillips R., Kondev J., Theriot, J. and Orme N. "Physical Biology of the Cell", Garland Science, 2005.

Note: Class notes would be provided.

CL 641	Process Intensification and Integration	(3-0-0-6)
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Preamble:

Due to environmental concerns, the need for more efficient and effective processes is increasing day by day to minimize waste production and energy consumption in a particular process. These issues can effectively be addressed by the use of process intensification and process integration concepts. By utilization of such systems one can also ensure the process safety. This course will introduce the concepts of process intensification and integration strategies to enhance the efficiency and cost effectiveness of a process as compared to its conventional counterparts. Knowledge of such advanced processes and their applications in industry are highly beneficial for chemical engineering students.

Course content:

Basic concepts and definitions; advantages of process intensification and integration; microstructured and monolithic reactors; multi-functional reactors: reactive distillation, reactive extraction, combined reaction and heat transfer; process intensification applied to various unit operations; process integration concepts: integration of microstructured devices (such as micro-reactors, micro-heat exchangers, micro-evaporators, micro-separators, etc.); industrial applications of these techniques: reactive distillation esterification, Desulfurization using catalytic distillation, microstructured reactors for phthalic anhydride synthesis and for flow chemistry (fine chemicals production).

Texts/Reference books:

1. D. Reay, C. Ramshaw and A. Harvey, Process intensification: engineering for efficiency, sustainability and flexibility, (1st Ed.) Butterworth-Heinemann, Burlington, 2008
2. A. Stankiewicz and J.A. Moulijn (Editors); Re-engineering the chemical processing plant: process intensification; Marcel Dekker, New York, 2004.
3. K. Boodhoo and A. Harvey (Editors) Process intensification for green chemistry: engineering solutions for sustainable chemical processing; John Wiley, West Sussex, 2013
4. F.J. Keil (Editor) Modeling of process intensification; Wiley-VCH verlag, 2007
5. R. Smith, Chemical Process: Design and Integration, (8th Ed.) John Wiley & Sons, Chichester, 2005

CL 642	Advanced Flow Measurement Techniques	(2-0-2-6)
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Preamble:

With the rapid progress in the electronics in last few decades, the flow measurement techniques have become accurate and it has become possible to acquire local pressure, temperature and velocity data with very high spatial and temporal resolutions. These techniques are not only being used for research purposes but also being increasingly used by the industry to validate CFD simulations and design more efficient devices, equipment and vehicles. This course aims to introduce the final year undergraduate and graduate-level students with the advanced flow measurement techniques along with the hands on experience in the use and post-processing of data obtained from such techniques.

Prerequisites: An undergraduate level course in fluid mechanics.

Course Content:

Conventional flow measurement techniques: Pitot tube, hot wire anemometry, flow meters; Flow Visualisation: Lasers, CCD and CMOS cameras, basics of filters, microscopy, fluorescence imaging; Digital signal and image processing: time series analysis, Fourier transforms, probability density function, auto- and cross correlations, correlation functions and their use in experiments; Fundamentals of Particle Image Velocimetry (PIV): Components of a basic PIV system, particle seeding, synchronization of laser and camera, post processing of PIV images; Advanced PIV techniques: micro-PIV, stereo-PIV, particle tracking velocimetry (PTV), time-resolved PIV, volumetric PIV; Laser induced fluorescence: Temperature and concentration measurements; Post-processing of PIV data: Contours, vectors, streamlines, shear stress, mean and fluctuating velocities in turbulent flows; Radiotracer-based flow measurement techniques: radioactive particle tracking (RPT); Phase distribution measurement: gamma ray densitometry; electrical capacitance tomography, electrical resistance tomography, electrical impedance tomography; Magnetic resonance imaging (MRI); Laser Doppler anemometry (LDA).

Text and Reference Books:

1. Dyke, M. van, An album of fluid motion, The Parabolic Press, 1982.
2. Chaouki, J., Larachi, F., and Dudukovic, M. P., Non-invasive Monitoring of Multiphase Flows, Elsevier Science Ltd., 1997.
3. Yang, W. J., Handbook of Flow Visualization, CRC Press, 2001.
4. Raffel, M., Willert, C.E., Wereley, S. and Kompenhans, J. "Particle Image Velocimetry: A Practical Guide", Springer, Second Edition, 2007.
5. Lee, T.-W., Thermal and Flow Measurements, CRC Press, 2008.
6. Adrian, R. J. and Westerweel, J. "Particle Image Velocimetry", Cambridge Aerospace Series, First Edition, 2011.

CL 643

Computer Aided Applied Optimization

(2-0-2-6)

Preamble:

Optimization problems are encountered in every discipline and a knowledge of optimization techniques can significantly aid researchers and practitioners alike. The course incorporates the application aspects of both meta-heuristic and mathematical programming techniques thereby enabling the students to judiciously choose the appropriate technique for their problem. The course will also lay special emphasis on the appropriate modelling that is required for solving a problem with either mathematical programming technique or meta-heuristic optimization algorithms through three case studies published in literature. Another unique feature of this course would be the hands-on sessions with three state-of-the-art tools for solving optimization problems which will enable the students to quickly set up and solve their problems as well as in implementing their own techniques and compare with other techniques. The choice of the software is made such that most types of optimization techniques are available in at least one of the tools discussed in this course. The course would also contain a project component in which the students can choose one or more of the following activities (i) formulate and solve an unsolved optimization problem of their choice, (ii) propose a single objective optimization technique, (iii) propose a technique to extend single objective optimization algorithms to solve multi-objective optimization problems, (iv) rigorously evaluate the performance of single or multi-objective algorithms that have been proposed in the previous year, (v) extend the single objective algorithms proposed in the previous year to solve multi-objective optimization problems, and (vi) performance metrics for analysing the diversity and convergence of MOEA.

Course Contents:

Introduction to Optimization; Single objective optimization algorithms: Sanitized Teaching Learning Optimization, Artificial Bee Colony Optimization, Particle Swarm Optimization, Differential Evolution, Simulated Annealing, Real Coded Genetic Algorithm with Simulated Binary Crossover and Polynomial Mutation; Constraint handling: penalty and constraint domination approach; Multi-objective optimization: Introduction, Strength Pareto Evolutionary Optimization, Non-dominated sorting & crowding distance, Epsilon domination based multi-objective optimization, Reference-point-based-many objective optimization; Extension of single objective optimization algorithms to multi-objective optimization; Hybridization and variants of optimization techniques; Mathematical programming techniques: Introduction, Simplex method, Branch & Bound, Sequential quadratic programming, Techniques to convert multi-objective optimization problems to single objective optimization problems; Introduction to Constraint Programming; Single and multi-objective optimization problems of Congress on Evolutionary Computation and The Genetic and Evolutionary Computation Conference; Case Studies: Production planning, Job shop scheduling, and Assignment of reviewers; Introduction to optimization tools: MATLAB/SCILAB, GAMS & NEOS Solver, IBM ILOG CPLEX Optimization Studio.

Text and Reference Books:

1. Rao, S. S., Optimization: Theory and Applications, 4, Wiley India, 2014,
2. Deb, K., Multi-objective Optimization using Evolutionary Algorithms, 1, Wiley India, 2010
3. Price, K., Storn, R., and Lampinen, J., Differential Evolution - A Practical Approach to Global Optimization, Natural Computing Series, Springer, 2005
4. Deb, K., Mohan, M., Mishra, S., Evaluating the epsilon domination based Multi-Objective Evolutionary Algorithm for a Quick Computation of Pareto-Optimal Solutions, Evolutionary Computation, MIT Press, 13 (4), 2005, 501-525
5. Deb, K., Jain, H., An Evolutionary Many-Objective Optimization Algorithm Using Reference-Point-Based Nondominated Sorting Approach, Part I: Solving Problems with Box Constraints, IEEE Transactions on Evolutionary Computation, 18 (4), 2014, 577 – 601
6. Rao, R.V., Savsan, V. J., Vakharia, D. P., Teaching-learning-based optimization: an optimization method for continuous non-linear large scale problems, Information Sciences, 183, 2012, 1-15
7. Janak, S.L., Taylor, M. S., Floudas, C. A, Burka, M., and Mountziaris, T. J., Novel and Effective Integer Optimization Approach for the NSF Panel-Assignment Problem: A Multiresource and Preference-Constrained Generalized Assignment Problem, Industrial & Engineering Chemistry Research, 45 (1), 2005, 258–265
8. Jain, V., Grossmann, I.E., Algorithms for Hybrid MILP/CP Models for a Class of Optimization Problem, INFORMS Journal on Computing, 13 (4), 2001, 258–276
9. Alfares, H.K., Al-Amer, A.M., An optimization model for guiding the petrochemical industry development in Saudi Arabia, Engineering Optimization, 2002, 34, 671 – 687

10. Črepinšek, M., Liu, S., Mernik, L., A note on teaching–learning-based optimization algorithm, Information Sciences, 2012, 212, 79 –93
11. Mernik, M., Liu, S., Karaboga, D., Črepinšek, M., On clarifying misconceptions when comparing variants of the Artificial Bee Colony Algorithm by offering a new implementation, Information Sciences, 2015, 291, 115 - 127

- (i) The journal articles are mandatory as part of reference as these describe some of the recent developments which have been incorporated in the syllabus but is not described in any of the books.
- (ii) Additionally, there are articles, which emphasize on appropriate strategies to be used to compare competing algorithms and common misconceptions and common pitfalls in reporting algorithms.
- (iii) Three of the journal articles are used as case studies, which can be used to explicitly show the advantages and disadvantages of the two broad categories of optimization techniques.
- (iv) The content in the journal references contribute to the uniqueness of the course and is not taught in most optimization courses nor is detailed in the books. Hence, these journal references are required for the course and need to be part of the syllabus.

CL 644	Petroleum Reservoir Simulation	(3 0 0 6)
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Preamble:

Reservoir simulation has become a necessary tool for the petroleum engineers, geologists, and subsurface modelers to predict future performance of the reservoir and find ways and means of optimizing the recovery of some of the hydrocarbons under various operating conditions. With the advances in computing capabilities and the numerical methods, the complex geological systems and mixtures of fluids can be tracked and visualized using the scientific computations. Insights from these simulations are expected to help in managing the reservoir assets and making reliable predictions about production rates.

In this course, the fundamental governing equations as well as the numerical techniques to discretize them will be covered. Simple linear algebra solvers will also be presented to enable building a simulator that can provide the hands-on implementation of ideas in reservoir management.

Prerequisites: NIL

Syllabus:

1. Overview of Petroleum Reservoir Engineering: Summary of rock and fluid properties, governing equations.
2. Introduction to Reservoir simulation: Reservoir simulation in petroleum engineering activity, Reservoir simulation method, Classification of models in reservoir simulation: single phase models, two-phase flows, black oil model, compositional model, thermal model, Commercial reservoir simulators.
3. Fundamentals of numerical discretization methods: Partial differential equations (PDEs), discretization, Taylor series, first and second derivative approximation, Finite difference, implicit and explicit, Linear algebra solvers.
4. Single Phase Flow and Numerical Solutions: Numerical solutions of basic differential equations for single flow.
5. Fundamentals of Multiphase Flow through Porous Media and Numerical Solution: Basic governing equations, two phase flow; oil-water simulations –IMPES solutions, saturated and under-saturated oil-gas simulations.
6. Well Modeling: Well index. Single -layer and multilayer well models, boundary conditions on the well. Peaceman's condition.
7. Introduction to Black oil and Compositional model, non-Isothermal Reservoir Simulation.
8. Simulation of fractured reservoirs, Upscaling, Streamline Simulations, Near Wellbore Flow Physics

Text and Reference Books:

1. Chen, Zhangxin, Reservoir Simulation: Mathematical Techniques in Oil Recovery. SIAM (2007)
2. K. Aziz, A. Settari, Petroleum Reservoir Simulation. Applied Science Publisher (2006).
3. Turgay Ertekin, J.H. Abou-Kassem, and G.R. King, Basic Applied Reservoir Simulation. Society of Petroleum Engineers (2001).
4. Peaceman, Donald W. Fundamentals of Numerical Reservoir Simulation. Elsevier (1977).

CL 645	Applied Statistics for Chemical Engineers	(3-0-0-6)
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Pre-Requisite: Nil

Preamble: A sound knowledge of statistics is essential for a chemical engineer. It is required in the applications such as curve fitting, stochastic modeling and optimization, and quality control. Conventional courses on mathematics and numerical methods do not cover this subject. In addition, a good exposure to the use of software (such as MATLAB and MINITAB) for the statistical computations is essential. This course attempts to fulfil these requirements.

Course Content/Syllabus:

Probability theory. Random variables. Variation plots. Probability distributions. Sampling and estimation theories. Hypothesis testing. Curve fitting. Analysis of variance. Stochastic modeling and simulation: random walk, Bernouli, Wiener, Poisson, Markov, Martingale, Lévy, and point processes, and Monte Carlo simulation. Statistical quality control: statistical process control and capability analysis, and design of experiments. Use of MATLAB's Statistics and Machine Learning Toolbox, and MINITAB for the solution of chemical engineering problems.

References:

1. M. R. Spiegel, J. J. Schiller, R. A. Srinivasan, and D. Goswami, Probability and Statistics, McGraw-Hill Education, 2017.
2. W. Volk, Applied Statistics for Engineers, Literary Licensing, 2013.
3. D. C. Montgomery, Statistical Quality Control, Wiley, 2015.
4. P. Mathews, Design of Experiments with MINITAB, New Age International, 2010.
5. N. G. Van Kampen, Stochastic Processes in Physics and Chemistry, North Holland, 2007.
6. M. Pinsky and S. Karlin, An Introduction to Stochastic Modeling, Academic Press, 2011.