M.Tech and PhD

Program Course Curriculum

Department of Chemical Engineering

Indian Institute of Technology Jodhpur

M.Tech. in Department of Chemical Engineering

Course Structure: Semester wise distribution of credits

Cat.	*Course Number, Course Title*		*L-T-P*	*Credits*		*Cat.*	*Course Number, Course Title*		*L-T-P*	*Credits*
I Semester						**II Semester**				
C	CHL7XX0	Advanced Mathematical Methods in Chemical Engineering	3-0-0	3		C	CHL7XX0	Advanced Thermodynamics	3-0-0	3
C	CHL7XX0	Advanced Reaction Engineering	3-0-0	3		E	CHL7XX0	*Elective-2*	3-0-0	3
C	CHL7XX0	*Advanced Transport Phenomena*	3-0-0	3		E	CHL7XX0	*Elective-3*	3-0-0	3
E	CHL7XX0	Elective-1	3-0-0	3		E	CHL7XX0	*Elective-4*	3-0-0	3
NG1	HSN7XX0	Non-Graded I	1-0-0	S/X		NG2	HSN7XX0	*Non-Graded II*	1-0-0	S/X
			Total	**12**					*Total*	**12**
III Semester						**IV Semester**				
T	CHT8XXo	Thesis		16		T	CHT8XX0	Thesis		16
			Total	**16**					*Total*	**16**

List of Electives

S.No.	Course Number	*Course Title*		
1.	CHL7XX0	Advanced Wastewater Treatment	3-0-0	3
2.	CHL7XX0	Chemometrics	3-0-0	3
3.	CHL7XX0	Computational Fluid Dynamics	3-0-0	3
4.	CHL7XX0	Heterogeneous Catalysis and Catalytic Reactors	3-0-0	3
5.	CHL7XX0	Modeling of atoms, molecules and surfaces	3-0-0	3
6.	CHL7XX0	Molecular Simulations	3-0-0	3
7.	CHL7XX0	Nanocomposite Membrane Technology	3-0-0	3
8.	CHL7XX0	Novel separation processes	3-0-0	3
9.	CHL7XX0	Principles of Electrochemical Engineering	3-0-0	3
10.	CHL7XX0	Process Optimization	3-0-0	3
11.	CHL7XX0	Process Safety & Hazards	3-0-0	3
12.	CHL7XX0	Structure & Property for Polymers	3-0-0	3

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S.No.	Category	Course Category Title	Total Courses	Total Credits
1	C	*COMPULSORY*	4	12
2	E	*ELECTIVES*	4	12
3	NG	*Non-Graded*	2	0
3	T	Thesis	**2 (16+16)**	32
		Total		**56**

Ph.D. program in the Department of Chemical Engineering

Course (Credit) Requirements for PhD students

S.No.	Ph.D. in	With	Minimum courses required	Total credits
1.	Engineering discipline	M.Tech., M.E. or M.Sc. (Engineering) in an Engineering discipline	4 Compulsory	**12**
		M.Sc. degree in a Science discipline	4 Compulsory (Same as M.Tech. Compulsory) + 4 Electives	**24**
		B.Tech., B.S., B.E. or B.Sc. (Engineering) in an Engineering discipline	4 Compulsory (Same as M.Tech. Compulsory) + 4 Electives	**24**

Doctoral compulsory (DC)	Electives
• Advanced Mathematical Methods in Chemical Engineering • Advanced Thermodynamics • Advanced Reaction Engineering • Advanced Transport Phenomena	PG elective list

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Detailed Course Contents

Course Title	**Advanced Mathematical Methods in Chemical Engineering**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	M.Tech., Ph.D.	Type	Compulsory
Prerequisite	None		

Objective

To familiarize the students with techniques of solving mathematical equations relevant to process engineering operations, and equip them with the underlying theoretical foundations of mathematical methods.

Learning Outcomes

The students will be able to

- solve linear and nonlinear algebraic equations, ordinary differential equations and partial differential equations using analytical and numerical techniques.
- analyse and comment on the solvability of single and system of simultaneous equations.
- identify mathematical models in process operations, and map them to appropriate solution techniques for solving and analyzing them.

Contents:

Linear algebra and numerical analysis

- Concept of linearity and operator algebra (2 lectures)
- Linear vector spaces: Linear independence, basis, dimension, span, simultaneous algebraic equations, null and range space (8 lectures)
- Inner product spaces, norm and metric spaces, adjoint operators, orthonormalization (4 lectures)
- Background and need for numerical analysis; review of numerical solutions of simultaneous linear and non-linear algebraic equations (2 lectures)
- Numerical solution of ODE-IVP’s including simultaneous equations, analysis of stability and convergence (2 lectures)
- Concept of discretization, numerical solution of ODE-BVP’s and PDE’s (2 lectures)

Differential equations

- Solution of simultaneous autonomous linear equations, bifurcation and linear stability analysis (3 lectures)
- Solution of non-autonomous equations (3 lectures)
- Sturm-Liouville theory; Frobenius solution of equations with variable coefficients (3 lectures)
- Classification of PDE’s; solution of PDE’s using separation of variables (4 lectures)
- Techniques for solution of PDE’s with non-homogeneous boundary conditions (6 lectures)

Text Books

1. Pushpavanam S., Mathematical Methods in Chemical Engineering (1st Ed.), PHI Learning, New Delhi 1998.
2. Logan D.J., *Applied Partial Differential Equations* (3rd Ed.), Springer International Publishing Switzerland 2015.
3. Gupta S.K., Numerical Methods for Engineers (1st Ed.), New Age International (P) Ltd., New Delhi 1995.

Reference Books

1. Davis M.E., Numerical Methods and Modeling for Chemical Engineers (1st Ed.), John Wiley and Sons, New York 1984.
2. Rice R.G., Do DD., Applied Mathematics and Modeling for Chemical Engineers (1st Ed.), John Wiley and Sons, New York 1995.

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Advanced Thermodynamics**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	M.Tech., Ph.D.	Type	Compulsory
Prerequisite	None		

Objective

To provide the students with knowledge and tools of classical and molecular thermodynamics with applications to chemical systems, and develop the importance and appreciation of the two approaches to the study of thermodynamics.

Learning Outcomes

The students will be able to

- carry out thermodynamic analysis of chemical systems to develop structure-property relationships.
- establish correspondence between bulk and molecular properties of materials.
- carry out thermodynamic calculations for multiphase and multicomponent systems.

Contents

Classical thermodynamics

- Review of classical thermodynamics, laws of thermodynamics, ideality in gases, non-ideal gas laws (2 lectures)
- Multicomponent thermodynamics, chemical potential, Maxwell's relations for multicomponent systems (3 lectures)
- Non-ideal gas and liquid mixtures, fugacity and activity, UNIFAC and UNIQUAC models for activity coefficient (6 lectures)
- Multiphase systems, analysis of stability of phases, two-phase and three-phase diagrams, multiphase-multicomponent systems, critical phenomena (6 lectures)

Molecular and statistical thermodynamics

- Fundamentals of statistical mechanics, statistical origins of second law of thermodynamics, Boltzmann entropy equation, ensembles, partition function, thermodynamic relations in different ensembles (6 lectures)
- Time-dependent and time-independent Schroedinger equation, solution of time-independent Schroedinger equation under various external potentials (4 lectures)
- Molecular partition function, determination of molecular energies with different degrees of freedom, correspondence with classical properties, reaction equilibrium and mixture properties (6 lectures)
- Kinetic theory of gases, mean free path, average speed calculation, random walk and diffusion, calculation of transport properties and introduction to non-equilibrium thermodynamics; molecular simulation techniques (6 lectures)

Text Book

1. Sandler S., *Chemical, Biochemical, and Engineering Thermodynamics* (5th Ed.), Wiely and Sons, New York 2017.
2. McQuarrie D.A., *Statistical Mechanics* (1st Ed.), Viva Books Pvt. Ltd.

Reference Books

1. Tester J.W., Modell M., *Thermodynamics and Its Applications* (3rd Ed.), Prentice Hall PTR, New Jersey 1997.
2. Callen H., *Thermodynamics and an Introduction to Thermostatistics* (2nd Ed.), John Wiely and Sons, New York 1991.
3. Denbigh K.G., *The principles of chemical equilibrium: With Applications in Chemistry and Chemical Engineering* (4th Ed.) Cambridge University Press, 1981

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Title	**Advanced Reaction Engineering**	Number	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 (3)
Offered for	M.Tech., Ph.D. in Chemical Engineering	Type	Compulsory
Prerequisite	None		

Objective
The Instructor will:
- Impart knowledge of hydrodynamics and transport effects in multiphase reactors, to learn lower order models for prediction of their performance.
- Introduce industrial reactors,
- Provide methodology to design multiphase reactors for a few specific applications.

Learning Outcomes
The students are expected to have the ability to
- In-depth understanding of hydrodynamics and transport effects in multiphase Reactors.
- Design multiphase reactors.

Contents
Reaction kinetics and ideal reactors: Review of reaction kinetics and ideal reactors, catalytic reactions, non-catalytic reactions (3 lectures)

Non-ideal reactors: Principles of non-ideal flow, central volume principle and RTD theorems, data analysis and interpretation; Models for non-ideal flow patterns, tanks in-series (8 lectures)

Non-isothermal reactor design: Energy balance for non-isothermal reactor, design of adiabatic reactors, impact on equilibrium conversion, design of tubular reactor with heat exchanger, mixed flow reactor with heat effect, multiple steady state (4 lectures)

Reaction Stability Analysis: Application of conformal mapping for identification of unique steady state and the criteria for the same; linear stability analysis. (3 lectures)

Fluid-Solid Non-Catalytic Reactions: Progressive conversion model, Shrinking core model, Gas film diffusion control, Ash layer diffusion control, Surface reaction control (3 Lectures)

Fluid-Solid Catalytic Reactions: Introduction to the basics of solid catalysts, Steps in catalytic reactions, Derivation of rate law for heterogeneous reaction, External mass transport limitations, Thiele Modulus, Effectiveness factor, Falsified Kinetics (6 Lectures)

Advanced Reactor Analysis:
Packed Bed Reactor: Classification of reactor models, Graphical design of non-isothermal reactor, pseudo homogenous models for reactor design (3 lectures)

Fluidized Bed Reactor: Introduction, Regimes of fluidized bed reactor, parameters for reactor design, models for reactor design, Kuni Levenspiel Model (4 lectures)

Slurry Bed and Trickle Bed Reactor: Different regimes of fluid flow, mass transfer coefficient, slurry bed models, trickle bed models (3 lectures)

Membrane Reactors: Types, transport mechanism, case study for H_2 production (2 lectures)

Text Books

1. Froment, G. F., K. B. Bischoff, 1990, *Chemical Reactor Analysis and Design*, John Wiley.
2. Doraiswamy, L. K. and D. Uner, 2013, *Chemical Reaction Engineering: Beyond the Fundamentals,* CRC Press.
3. J.M. Smith: 1981, Chemical Engineering Kinetics, McGraw Hill, Third Edition.

Reference Book

1. Carberry, J. J., Varma, A., 1986, *Chemical Reaction and Reactor Engineering*, Marcell-Dekker

Online Course Material

1. Shankar, H.S., Advanced Chemical Reaction Engineering, NPTEL Course Material, Department of Chemical Engineering, IIT Bombay, https://nptel.ac.in/courses/103/101/103101001/
2. Viswanathan, G.A., Chemical Reaction Engineering II, NPTEL Course Material Department of Chemical Engineering, IIT, Bombay, https://nptel.ac.in/courses/103/101/103101008/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Advanced Transport Phenomena**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	M.Tech., Ph.D.	Type	Compulsory
Prerequisite	None		

Objective

The instructor will:

- Provide in-depth understanding of processes involving mass, energy, and momentum transport.

Learning Outcomes

The students are expected to have the ability to:

- Understand the fundamental aspects of transport phenomena at advanced level.
- Develop an understanding and pursue graduate research in this area

Contents

Introduction: Review of fluid kinematics, Control Volumes, Reynolds transport (**4 lectures**)

Conservation Principles and constitutive laws: Mass, Momentum, Energy, Entropy; Phase interface conditions, Solutions methods for equations of change, steady and unsteady fluid flow, Creeping flow, Lubrication approximation, Boundary layer theorem (**12 lectures**)

Coupled transport processes: Steady and Unsteady states phenomena, Forced convection heat and mass transport in confined/unconfined laminar flows, low Peclet and high Peclet approximations, buoyancy driven flows, Multi-component energy and mass Transport. (**12 lectures**)

Turbulence modelling: Characteristics of turbulent flows, length and time scales, energy cascade, Reynolds averaged transport equations, Phenomenological models, Kolmogorov hypotheses, universality and turbulence spectra (**10 lectures**)

Transport phenomena in large-scale and small-scale systems: chemical reactors, micro-fluidic devices (**4 lectures**)

Text Book

1. Deen W. M., 1998, Analysis of Transport Phenomena, Oxford University Press, New York.
2. Bird. R. B., Stewart, W. E. and Lightfoot, E. N., 2006, Transport Phenomena, 2nd edition, John Wiley & Sons.

Reference Books

1. Slattery J.C., 1999, Advanced Transport Phenomena, Cambridge University Press.
2. Leal L. G., 2010. Advanced Transport Phenomena: Fluid mechanics and convective transport processes, Cambrige University Pres.
3. Pope S. B., 2000, Turbulent Flows, Cambridge University Press.
4. Belfore, L. A., 2003, Transport Phenomena for Chemical Reactor Design, John Wiley & Sons.
5. Ramachandran, P. A. 2014. "Advanced Transport Phenomena", Cambridge University Press.

Online Course Material

1. R. Nagarajan, Advanced Transport Phenomena, NPTEL Course Material, Chemical Engineering, IIT Madras, https://nptel.ac.in/courses/103106068/#
2. V. Kumaran, Fundamentals of Transport Processes, NPTEL Course Material, Department of Chemical Engineering, IIsc Bangalore, https://nptel.ac.in/courses/103/108/103108099/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Advanced Wastewater Treatment**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	None		

Objective

The instructor will:

- Impart comprehensive knowledge of industrial and municipal wastewater.
- Discuss mechanism and methodologies for wastewater treatment.
- Discuss case studies

Learning Outcomes

The students are expected to have the:

- Comprehensive knowledge of the wastewater treatment.
- Knowledge of advanced methodologies such as wastewater management, recycle and reuse.

Contents

Introduction: Wastewater engineering: an overview, characterisation of wastewater and monitoring of industrial and municipal wastewater, emerging contaminants, environmental impacts of wastewater constituents. (**4 lectures**)

Conventional Water/ Wastewater Treatment: Existing unit operations and processes, basic philosophy of water and wastewater treatment plants; physio-chemical treatment methods: (i) Screening, (ii) conventional filtration, (iii) coagulation, (iv) flocculation, (v) floatation, (vi) Clari-flocculation (vii) sedimentation, (viii) sand filtration, etc. (**10 lectures**)

Aerobic and Anaerobic Suspended and Attached Growth Wastewater Treatment Processes: Aerated lagoon, activated sludge systems, trickling filter, sequential batch reactor, fluidized bed bioreactors, Up-flow Anaerobic Sludge Blanket (UASB) and hybrid Up-flow Anaerobic Sludge Blanket (UASB) reactors. (**8 lectures**)

Advanced Treatment Processes: Membrane Filtration, microfiltration, ultrafiltration, nanofiltration, reverse osmosis, and electrodialysis; wet air oxidation, adsorption, and ion exchange; wet-land and root-zone treatment of industrial and municipal wastes; design of sludge drying beds, thermal and biological processes for sludge and land fillings. Membrane reactors, new technologies for wastewater disinfection. (**10 lectures**)

Water Recycling and Reuse: Different unit operations for water recycling depending on end use, energy considerations, recovery of valuables from wastewater, zero liquid discharge (ZLD). (**7 lectures**).

Text Book

1. Burton F.L., Tchobanoglous G., Stensel H.D., 2017, Waste Water Engineering Treatment and Reuse, 4th ed.,Tata McGraw-Hill.
2. Arceivala S.J. and Asolekar S.R., 2007, Wastewater Treatment for Pollution Control and Reuse, 3rd Ed., Tata McGraw Hill.

Reference Books

1. Henze M., van-Loosdrecht M.C.M., Ekama G.A. and Brdjanovic D., 2008, Biological Wastewater Treatment: Principles, Modelling and Design, IWA publishing.
2. Sincero A.P. and Sincero G.A., 1996, Environmental Engineering – A Design Approach, Prentice-Hall.
3. Tewari P.K., 2020, Advanced Water Treatment, CRC Press, Taylor and Francis Group (USA)

Online Course Material

1. Tiwari M K, Wastewater treatment and recycling, NPTEL course material, Department of Civil Engineering, IIT Kharagpur, https://nptel.ac.in/courses/105105178/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Chemometrics**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	basics of chemical engineering		

Objective

The instructor will:

- Impart knowledge of modern methods of analyzing chemical data.

Learning Outcomes

The students are expected to have the:

- Comprehensive knowledge of the modern methods of reducing and analyzing chemical data.

Contents

Prelude to chemometrics: Introduction and history of Chemometrics, factorial analysis; reverse, surface and mixture design; correlograms and time series analysis; sequential methods, Pattern recognition. (**6 lectures**)

Calibration: introduction to multivariable calibration, selectivity problems, statistical problems in calibration, Univariate calibration, multiple linear and principal components regression, model validation, outlier detection. (**6 lectures**)

Evolutionary signals and process analysis in chemical plants: exploratory data analysis and processing, determining composition, resolution pre-processing, composition of sequential data, screening. (**6 lectures**)

Derivatives in Spectroscopy: Theoretical and computed derivatives, derivative approximation, calibrating with derivatives, spectroscopic monitoring of reactions, kinetics and multivariable model, online spectroscopy. (**6 lectures**)

General Data Analysis: simple analysis of variance and experimental design (one-way, two-way with and without replicates, randomized and blocked designs). (**6 lectures**)

Computational methods: control structures for selection and iteration, functions, array data structure, numerical methods for data analysis. (**6 lectures**)

Machine learning in Chemical plants: Introduction, basics of decision trees, combining multiple learner, reinforcement learning, experimental design and analysis. (**6 lectures**)

Text Book

1. Richard G. Brereton, 2003, Chemometrics: Data Analysis for the Laboratory and Chemical Plant, Wiley

Reference Books

1. Harald Martens, Tormod Næs, 1989, Multivariate Calibration, John Wiley & Sons.
2. Howard Mark, Jerry Workman, Jr, 2018, Chemometrics in Spectroscopy, Elsevier Academic Press.

3. Richard G. Brereton, 2007, Applied Chemometrics for Scientists, John Wiley & Sons.
4. Ethem Alpaydin, 2004, Introduction to Machine Learning, MIT Press.
5. Vandeginste, B.G.M., Massart, D.L., Buydens, L.M.C., Jong, de D., Lewi, P.J., Smeyers- Verbeke, J., 1998, Handbook of Chemometrics and Qualimetrics: Part B, Elsevier.
6. Kreyszig, Erwin, 2014, Advanced Engineering Mathematics, John Wiley and Sons, 10th Edition.

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Computational Fluid Dynamics**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	None		

Objective

The Instructor will:

- Impart knowledge about various computational methods of fluid flow and heat transfer.
- Provide insight to design and simulate the hydrodynamics and multi-physics systems.

Learning Outcomes

The students are expected to have the ability to

- In-depth understanding of numerical methods for solution of partial differential equations of fluid flow and heat transfer.
- Acquire knowledge of grid generation, processing and applications of CFD.

Contents

Introduction: Fundamental principles of conservation, Reynolds transport theorem, conservation of mass, conservation of linear momentum: Navier-Stokes equations, conservation of energy, Mathematical classification of partial differential equations, physical, boundary conditions. (**8 lectures**)

Finite Difference Method (FDM): Discretization of ODE and PDE, approximation for first, second and mixed derivatives, implementation of boundary conditions, discretization errors, grid generation, uniform vs non-uniform grids, Discretization of unsteady diffusion problems: Explicit, Implicit and Crank-Nicolson's algorithm; stability of solutions, stream function - vorticity approach, Poisson equation (**12 lectures**)

Finite Volume Method (FVM): Discretization methods, approximations of surface integrals and volume integrals, Modelling of Convection- Diffusion Problems: One dimensional convection-diffusion problem: Central difference scheme; Discretization based on analytical approach (exponential scheme); Hybrid and power law discretization techniques; Higher order schemes (QUICK algorithm) (**10 lectures**)

Flow modeling: Discretization of incompressible flow equations; Pressure based algorithm: SIMPLE, SIMPLER etc; Unstructured grids; Introduction to turbulence modeling; Large Eddy Simulation (LES); Direct Numerical Simulation (DNS) (**9 lectures**)

Text Book

1. Anderson J.D., 1995, Computational Fluid Dynamics, McGraw Hill.
2. Ghoshdastidar P.S., 1998, Computer Simulation of Flow and Heat Transfer, Tata McGraw Hill.
3. Patankar, S. . Numerical Heat Transfer and Fluid Flow. Mcgraw Hill, 2017

Reference Books

1. Fletcher C.A.J., 1998, Computational Techniques for Fluid Dynamics, Vol. 1: Fundamental and General Techniques, Springer-Verlag.
2. Fletcher C.A.J., Computational Techniques for Fluid Dynamics, 1998, Vol. 2: Specific Techniques for Different Flow Categories, Springer-Verlag.
3. Ferziger J.H. and Peric M., 2002, Computational Methods for Fluid Dynamics, 3rd Ed., Springer

Online Course Material

1. Jayanti, S., Computational Fluid Dynamics, NPTEL Course Material, Department of Chemical Engineering, IIT Madras, https://nptel.ac.in/courses/103/106/103106119/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Heterogeneous Catalysis and Catalytic Reactors**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	Basic knowledge of Chemical Kinetics		

Objective

The Instructor will:

- Impart knowledge about the basic concepts, detailed structures, preparation methods and reactivities of solid catalysts, its properties and relationship between the structures and reactivities.

Learning Outcomes

The students are expected to have the ability to:

- Understand and gain knowledge of the detailed structures, preparation methods and reactivities of solid catalysts, its properties and relationship between the structures and reactivities.

Contents

Introduction to basic concepts (**2 lectures**)

Catalysis: Acid-base catalysis, application of catalyst functionality concepts for control of reaction selectivity and kinetic models, Properties of catalysts, reaction selectivity and kinetic models (**10 lectures**)

Steps in catalytic reaction: Adsorption, Kinetic models, intraparticle transport process, Selection and design of catalysts, Preparation and characterization of catalysts, Catalyst deactivation, various deactivation models, Optimal distribution of catalyst in a pellet (**14 lectures**)

Zeolites: Preparation and characterization of various Zeolite catalysts and their application (**4 lectures**)

Commercial Reactors and catalysts: Adiabatic, fluidized bed, trickle bed, slurry; industrially important catalysts, Environmental catalysis (**8 lectures**)

Design of Catalytic Reactors for gas and two phase systems, Design of polymeric reactors. (**4 lectures**)

Text Book

1. Sharma M.M. and Doraiswamy, Heterogeneous Reactions, Vol 1 and Vol II
2. Thomas, J.M., Thomas W.J., Principles and practice of heterogeneous Catalysis.
3. I. Chorkendorff, J.W Niemantsverdriet., Concept of Modern Catalysis and Kinetics, 3rd Edition, Wiley VCH

Reference Books

1. Bruce Gates , Catalytic Chemistry.
2. Morbidelli and Verma , Optimal distribution of catalyst in a pellet.
3. Ford M.E. and Marcel Dekker, Catalysis of Organic reactions.

Online Course Material

1. Pant, K.K., Heterogeneous Catalysis and Catalytic Processes, NPTEL Course Material, Department of Chemical Engineering, IIT Delhi, https://nptel.ac.in/courses/103/102/103102012/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Modelling of Atoms, Molecules and Surfaces**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	Basic knowledge of Chemical Kinetics		

Objective

The Instructor will:

- Provide background on various forms of Intermolecular and Molecule-Surface interactions.

Learning Outcomes

The students are expected to:

- Gain fundamental understanding on the molecular nature of systems and surfaces.
- Learn about the importance of intermolecular forces in molecular modeling and simulations in chemical and allied engineering.

Contents

Introduction: Four Forces of Nature, Early Scientific Period (1 Lecture), First Phenomenological Theories, Modern View of origin of Intermolecular Forces (2 Lectures).

Forces Between Atoms and Molecules, Principle and Concepts: Some Thermodynamic Aspects of Intermolecular Forces (3 Lectures), Covalent and Coulomb Interactions (3 Lectures),

Interactions Involving Polar Molecules, Interactions Involving Polarisation of Molecules (5 Lectures), van der Waals Forces (3 Lectures), Repulsive Forces, Total Pair Potentials (3 Lectures), Hydrogen Bonding, Hydrophobic and Hydrophilic Interactions (2 Lectures).

Forces Between Particles and Surfaces: Concepts of Intermolecular and Interparticle Forces (2 Lectures), Contrast Between Intermolecular, Interparticle and Intersurface Forces (3 Lectures), van der Waals Forces Between Surfaces (2 Lectures), Electrostatic Forces Between Surfaces in Liquids (5 Lectures), Solvation, Structural and Hydration Forces (3 Lectures), Steric and Fluctuation Forces (3 Lectures), Adhesion (2 Lectures).

Text Book

1. J. N. Israelachvili, 2003, Intermolecular and Surface Forces, 2nd Edition, Academic Press.

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Molecular simulations**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	None		

Objective

To impart theoretical understanding and working solutions for modelling and simulation of molecular systems, and to be able to relate molecular structure and properties to bulk observables.

Learning Outcomes

The students will be able to

- model molecular systems with appropriate details needed for relevant simulation techniques.
- make appropriate choices of simulation techniques to suit the molecular system and the properties to be determined.
- develop theoretical understanding and carry out elementary simulations based on molecular dynamics simulations, Monte-Carlo simulations and density functional theory calculations.

Contents

Preliminaries

- Description of molecular systems, technique-appropriate system description of molecular systems (1 lecture)
- Overview of statistical mechanics, partition function and property estimation in different ensembles (2 lectures)

Molecular dynamic simulations

- Force-field description of molecular systems, coarse grain modelling, reactive force-fields (2 lectures)
- Algorithms for dynamical evolution of molecular systems, thermo- and barostats (4 lectures)
- Approaches to calculation of equilibrium and non-equilibrium transport properties, chemical potential and time-correlation and radial distribution functions (3 lectures)
- Analysis of data from molecular dynamics simulations with examples and case studies, including but not limited to, separation processes, adsorption, gas-gas separation, molecular sieves and membrane separation, protein simulations (3 lectures)

Monte-Carlo simulations

- Elementary statistical thermodynamics, bulk property estimation from partition function (3 lectures)
- Generation of microstates and identification of Monte-Carlo moves for different molecular systems, averaging of properties in different ensembles, Metropolis algorithm, enhanced sampling techniques (4 lectures)
- Average techniques, convergence and estimation of error with sampling (2 lectures)
- Analysis of data from Monte-Carlo simulations with examples and case studies, including but not limited to, nanotechnology, nanocrystals, defects, condensed matter simulations, applications to the analysis of novel materials (3 lectures)

Density functional theory calculations

- Introductory quantum mechanics and Schroedinger equation, description and solution of electronic structure of hydrogen (3 lectures)
- Motivation for techniques for many-body molecular problems, elementary theory of *ab initio* methods, Hohenberg-Kohn theorems, Kohn-Sham formulation, self-consistent field calculation, structural optimization (6 lectures)
- Analysis of data from DFT calculations with examples and case studies, including but not limited to, catalysis, surface process and adsorption, materials design (3 lectures)

Assignments will include small scripting and projects involving python or other suitable tools for continuous evaluation.

Textbook

1. Leach A.R., *Molecular Modelling: Principles and Applications* (2nd Ed.), Prentice Hall, New York 2001.

Reference Books

1. Jensen F., *An Introduction to Computational Chemistry* (2nd Ed.) John Wiely and Sons, West Sussex 2007.
2. Frenkel D., Smit B., *Understanding Molecular Simulation: From Algorithms and Applications* (1st Ed.), Academic Press, London 2002.
3. Landau D.P., Binder K., *A Guide to Monte Carlo Simulations in Statistical Physics* (3rd Ed.), Cambridge University Press, Cambridge 2009.

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Nanocomposite Membrane Technology**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	Basic knowledge of Engineering and Chemistry		

Objective

The instructor will provide:

- Fundamentals, synthesis and characterisation of nanocomposite membrane,
- Different applications of nanocomposite membrane technology.

Learning Outcomes

The students are expected to have:

- Comprehensive knowledge of fundamentals, synthesis and characterisation of nanocomposite membrane technology.
- Its applications in different fields such as water treatment, gas separation etc.
- Challenges and opportunities.

Contents

Introduction to nanocomposite membrane technology: Membrane types, membrane processes, transport theories. (**8 Lectures**)

Synthesis of nanocomposite membranes: Preparation techniques, homogeneous membranes, composite membranes, raw materials, processing methods. (**6 Lectures**)

Characterisation of nanocomposite membranes: Pore size, micrographic methods, spectroscopic methods, strength measurements. (**6 Lectures**)

Nanocomposite membranes in water treatment: Conventional nanocomposites, thin film nanocomposites, TFC with nanocomposite substrate. (**7 Lectures**)

Nanocomposite membranes in gas separation. (**5 Lectures**)

Challenges in processing of nanocomposite membranes. (**5 Lectures**)

Environment and safety issues. (**5 Lectures**)

Text Book

1. Tewari, P.K., (2016), Nanocomposite Membrane Technology: Fundamentals and Applications, CRC Press, Taylor & Francis Group.

Reference Books

1. Baker, R.W., (2004), Membrane Technology and Applications, 2nd Edition, Membrane Technology and Research Inc., Menlo Park, CA.

Online Course Material

1. Mohanty, K., Membrane Technology, NPTEL Course Material, Department of Chemical Engineering, IIT Guwahati, https://nptel.ac.in/courses/103/103/103103163/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Novel separation processes**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	Mass Transfer		

Objective

The Instructor will:

- Provide in-depth knowledge about the multi-component separation processes that are relevant to industries today.

Learning Outcomes

The students are expected to gain:

- Understanding of multicomponent separation processes with relevant industry examples and case studies.
- Gaining knowledge about the design of separation processes.

Contents

Fundamentals & Identification of separation process*:* Mass Diffusion, Fick's law, Separation factor, chemical potential, use of Navier-Stokes equation in mass transfer, Types of existing processes, equilibrium governed processes, rate governed processes **(6 lectures)**

Membrane-based separation processes: Fundamentals: Membrane casting, barrier types, Types of motion of molecules through the barrier, Categorization of membrane processes, osmotic pressure, observed vs real retention, estimation of retention and permeability, modules, Driving forces in membrane separation processes, Transports in Reverse Osmosis (RO), solution-diffusion model, concentration polarization and membrane fouling **(10 lectures)**

Membrane-based separation processes: Design and applications: Design of Membrane modules, Dialysis, Gas Separation by membranes , Electric field enhanced membrane filtration; (5) Electrophoretic Separation Processes **(7 lectures)**

Surfactant-based separation processes: Cloud point, mechanism of phase separation, ionic & non-ionic surfactants, volume reduction factor, partition coefficient, fractional coacervate volume, micellar enhanced ultrafiltration, liquid membranes **(7 lectures)**

Chromatographic separation processes: Chromatographic separation & ion exchange fundamentals, purpose of column, gas-liquid chromatography, liquid-liquid chromatography, involved processes, solute movement, ion exchange resin, ion movement theory **(3 lectures)**

Supercritical fluid extraction: critical condition, different supercritical fluids. Modifiers, methodology of SCF, solubility diagrams, Mollier diagrams **(4 lectures)**

Miscellaneous separation processes: Pervaporation, Membrane Distillation, etc. **(2 lectures)**

Text Book

1. Seader, Henley and Ropar (2011) Separation Process Principles, 3rd Edition Wiley.
2. W.S.W Ho and K. K. Sirkar, Membrane Handbook", Vol 1 and Vol 2;1992; Springer, https://doi.org/10.1007/978-1-4615-3548-5

Reference Books

1. Humphrey, J. L. and Keller, G. E., 1997, Separation Process Technology, McGraw- Hill, NY
2. Kister, H. Z., 1992, Distillation Design, McGraw-Hill.
3. Ross Taylor, R. Krishna, (1993) Multicomponent Mass Transfer, John Wiley & Sons.

Online Course Material

1. Dr. Sirshendu De Professor, Department of Chemical Engineering, IIT Kharagpur, NPTEL: Novel Separation Processes, https://archive.nptel.ac.in/courses/103/105/103105061/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Principles of Electrochemical Engineering**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	Basic knowledge of Thermodynamics		

Objective

The Instructor will:

- Provide the student with the essential knowledge needed to understand electrochemical engineering and technology.
- Illustrate the basic principles of electrochemistry, electrokinetic phenomena required for modelling and design of electrochemical processes and devices.

Learning Outcomes

The students are expected to have the ability to:

- Understand the principles of electrochemistry processes and electro-analytical methods.
- Correlate the principles of electrochemistry to electrochemical processes and suggest design solutions to engineering problems.

Contents

Basic Principles: Introduction to electrochemistry and fundamentals, Nernst equation, Electrode kinetics, Volta and Galvani potentials, electrochemical potential, electrochemical equilibrium, Enthalpy and Gibbs free energy calculation, solvation energy, ionic equilibrium. (**6 lectures**)

Cell potential: Electrochemical cell, standard electrode potential, Butler-Volmer formulation, Tafel equation, Pourbaix diagram, Activity Coefficients, Donnan potential, reversible electrode, Born model for ion-solvation energy, Batteries and Cell Chemistries. (**7 lectures**)

Ion-ion interactions and ionic transport: Debye-Huckel theory, activity coefficient of ionic solution, ion pair, Bjerrum theory and Fuoss theory, migration, extended Nernst-Planck equation, electrochemical mobility and its relation with diffusivity, Stokes-Einstein equation, ionic conductivity, transport number, Kohlrausch law. (**12 lectures**)

Charged interface: surface excess quantity, Lippmann equation, Gouy-Chapman model, Stern layer, internal and external Helmholtz layer, zeta potential, electric double layer. (**8 lectures**)

Electrochemical Kinetics: Nonequilibrium formulation, diffusion potential, junction potential, Planck-Henderson equation, pH electrode, electro-osmosis, electrophoresis, streaming potential, sedimentation potential. (**7 lectures**)

Application: Electro-chemical Processes, Fuel Cells. (**2 lectures**)

Text Book

1. Prentice ,G., 1991, Electrochemical Engineering Principles, Prentice Hall.

2. Girault, H., 2004, Analytical and Physical Electrochemistry, EPFL Press, 1st Edition.

Reference Books

1. Allen J. Bard, Larry R. Faulkner, 2005, Electrochemical Methods: Fundamentals and Applications, John Wiley & Sons; 2nd Edition.
2. Fuller,T.F., Harb, J. N., 2018, Electrochemical Engineering, Wiley.

Online Course Material

1. https://nptel.ac.in/courses/104106105/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Process Optimization**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	None		

Objective

The instructor will:

- Provide in-depth knowledge of various techniques of optimization and their application to chemical processes.

Learning Outcomes

The students are expected to:

- Have fair knowledge of various techniques of optimization and their application to chemical processes.

Contents

Introduction: Optimization and calculus based classical optimization Techniques (**4 lectures**)

One Dimensional Minimization Methods: Elimination methods- equally spaced points method, Fibonacci method and golden section method; Interpolation methods- quadratic interpolation and cubic interpolation, Newton and quasi-Newton methods, Linear Programming (**10 lectures**)

Multivariable Non-Linear Programming: Unconstrained- Different methods for non-linear programming; Constrained- complex method, feasible directions method, GRG method, penalty function methods and augmented Lagrange multiplier method. (**9 lectures**)

Dynamic Programming: Multistage processes- acyclic and cyclic, sub-optimization, principle of optimality and applications. (**6 lectures**)

Geometric Programming (GP): Differential calculus and Arithmetic-Geometric inequality approach to unconstrained GP; Constrained GP minimization; GP with mixed inequality constraints and Complementary GP, Emerging Optimization Techniques: Genetic algorithm, simulated annealing, particle swarm and ant colony optimization. (**10 lectures**)

Text Book

1. Edgar T.F., Himmelblau D.M. and Lasdon L.S., 2001, Optimization of Chemical Processes, 2nd Ed., McGraw Hill.

Reference Books

1. Beveridge G.S.G. and Schechter R.S., 1970, Optimization: Theory and Practice, McGraw Hill.
2. Rao S.S.,2009, Engineering Optimization Theory and Practice, 4th Ed., Wiley

Online Course Material

1. Sarkar, D., Optimization in Chemical Engineering, NPTEL Course Material, Chemical Engineering, IIT Kharagpur, https://nptel.ac.in/courses/103/105/103105139/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Process Safety & Hazards**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	Basic Knowledge of Chemical Engineering		

Objective

The Instructor will:

- Provide comprehensive knowledge of safety regulations and their practices, chemical plant hazards and their control, risk assessment and management principles and techniques and accident analysis.

Learning Outcomes

The students are expected to have the ability to:

- Identify and distinguish typical sources of risk and hazard in a process plant, undertake hazard and operability (HAZOP) study.

Contents

*Safety in Industries: Concepts and definition, storage of dangerous materials, Plant layout Safety systems, Occupational Safety and Health Administration (OSHA) incidence rate, Fatal accident rate (FAR), Measures to take during accidents, Toxicology (**10 lectures**)*

*Industrial Hygiene: Government regulations, Industrial hygiene and safety aspects related to toxicity, noise, pressure, temperature, vibrations, radiation etc, Evaluation Methods, Evaluating workers Exposures to dusts, noise. (**8 lectures**)*

*Selection Mechanism: Technology and process selection, Scale of disaster, Fire triangle Ignition, Confined and unconfined explosion, Vapors cloud explosions, Boiling liquid expanding vapor explosion (BLEVE), Dust explosion, shock wave, Flammability characteristics of liquids and vapors, Minimum oxygen concentration (MOC) and Inerting. (**8 lectures**)*

*Handling Chemicals and toxicity: Control of toxic chemicals, Storage and handling of flammable and toxic chemical, Runway reactions, Relief system risk and hazards management, Design to prevent Fires and Explosions, Miscellaneous Design for preventing Fires and Explosion. (**8 lectures**)*

*Hazards Identification: checklists, Surveys, Hazard and Operability Studies (HAZOP), Safety reviews. Risk Assessment, Hazard models and risk data. Tackling disasters, plan for emergency. Risk management routines, Emergency shutdown systems, Role of computers in safety, Prevention of hazard human element, Technology and process selection. (**8 lectures**)*

Text Books

1. Daniel A. Crowl and Joseph F. Louvar, 1990, Chemical Process Safety: Fundamentals with applications, Prentice Hall, Inc.
2. Lee, F.P., 1983, Loss prevention in the process Industries, Volume 1 and 2 Butterworth.
3. Hoboken, N. J., 2000, Guidelines for Chemical Process Quantitative Risk Analysis, Wiley-Interscience.

Reference Books

1. R. W. King and J. Magid, Industrial Hazards and Safety Handbook, Butterworth, 1982.

2. G. L. Wells, Safety in Process Plant Design, John Wiley and Sons Inc., 1980.
3. Fawcett, H.H. and W.S. Wood, Safety and Accident Prevention in Chemical Operations, 2nd Edition, Wiley-Interscience, New York, 1982.

Online Course Material

1. Sinha, S., Chemical Process Safety, NPTEL Course Material, Department of Chemical Engineering IIT Roorkee, https://nptel.ac.in/courses/103/107/103107156/

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

URL :- https://www.iitj.ac.in/chemical-engineering/en/curriculum

Course Title	**Structure & Property for Polymers**	Course No.	CHL7XX0
Department	Chemical Engineering	Structure (L-T-P [C])	3-0-0 [3]
Offered for	B. Tech., M.Tech., Ph.D.	Type	Elective
Prerequisite	An introductory course on polymers for B.Tech, None for M.Tech		

Objective

The Instructor will:

1. Provide knowledge about various structures in polymers and it's relation with the mechanical and thermal properties

Learning Outcomes

The students are expected to gain:

1. Understanding of structure-property for various polymeric systems
2. Understanding of thermal transition and deformation mechanisms in polymers

Contents

Introduction: Outline of the course, review of basics of polymers, polymerization reactions and classification (**2 lectures**)

Amorphous and Semicrystalline Polymers: Glass transition, free-volume theory, factors affecting glass transition temperature, solution grown single crystals and chain-folding mechanism, melt crystallization, spherulites, degree of crystallinity, Bragg's law, crystal thickness and chain extension, flow-induced crystallization, dimensionless numbers in crystallization, factors affecting melting, relationship between melting and glass transition (**11 lectures**)

Multicomponent Polymeric Systems: Polymer blends, block copolymers, thermoplastic elastomers, examples, phase diagram, glass transition, compatibilization, morphology diagram (**6 lectures**)

Deformation in Polymers: Elastic deformation, stress-strain relationship, polymer chain deformation, crystal moduli, elastic deformation in semicrystalline polymers, yield and crazing – necking and it's mathematical treatment, yield criteria, mechanisms, plastic deformation (**9 lectures**)

Viscoelasticity: Introduction, examples, Mechanical models, Boltzmann superposition principle, dynamic mechanical testing, transitions and polymer structure, t-T superposition, entanglements (**9 lectures**)

Polymer Composites: Matrix and fillers, composition, elastic deformation, fracture, packing, experiments, nanocomposites (**5 lectures**)

Text Book

1. Young R.J. and Lovell P.A. (2011) Introduction to Polymers, 3rd Edition, CRC Press

Reference Books

1. Chanda M. (2006) Introduction to Polymer Science & Chemistry, CRC Press

Online Course Material

1. Adhikari B, Science & Technology of Polymers, NPTEL Course Material, Department of Metallurgy & Material Science, Indian Institute of Technology Kharagpur, https://nptel.ac.in/courses/113105028/