DEPARTMENT OF CHEMICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY (INDIAN SCHOOL OF MINES), DHANBAD

COURSE STRUCTURE & SYLLABUS

FOR

Ph.D.

IN

CHEMICAL ENGINEERING

Effective from 2021-2022

Department of Chemical Engineering
Indian Institute of Technology (Indian School of Mines), Dhanbad

COURSE STRUCTURE
Ph.D. in Chemical Engineering

Option - II

First Semester (Monsoon)

Sl. No.	Course Code	Course Name	Course Type	L-T-P	Credit	Faculty Name	Employee Code
1	CHC501	Advanced Transport Phenomena	DC1	3-0-0	9		
2.	CHC502	Advanced Chemical Engineering Thermodynamics	DC2	3-0-0	9		
3.	CHC503	Computational Techniques in Chemical Engineering	DC3	3-0-0	9		
4.	CHC504	Advanced Chemical Reaction Engineering	DC4	3-0-0	9		
5.		Research and Technical Communication*	DC5	3-0-0	9 / (S/X)		
				Total Credit	**45/36**		

* Credit course for HSS scholars with 9 credit and Audit course (S/X) for others.

Second Semester (Winter)

Sl. No.	Course Code	Course Name	Course Type	L-T-P	Credit
1		Refer Basket for DE1	DE1	3-0-0	9
2.		Refer Basket for DE2	DE2	3-0-0	9
3.		Refer Basket for DE3/OE1	DE3/OE1	3-0-0	9
4.		Refer Basket DE4/OE2	DE4/OE1	3-0-0	9
5.	CHC518	Research Methodology	DC6	3-0-0	9
				Total Credit	**45**

Basket for DE1:

Sl. No.	Course Code	Course Name
1	CHD502	Nanotechnology
2.	CHD503	Catalysts & Materials Characterization Techniques

Basket for DE2:

Sl. No.	Course Code	Course Name
1	CHD504	Process Optimization
2.	CHD505	Interfacial and Colloidal Phenomena

Basket for DE3/OE1: OE1 (specify as DE or OE)

Sl. No.	Course Code	Course Name
1.	CHO501	Rheology
2.	CHO502	Fluidization Engineering

Basket for DE4/OE2: OE2 (specify as DE or OE)

Sl. No.	Course Code	Course Name
1.	CHO501	Rheology
2.	CHO502	Fluidization Engineering

Third Semester (Monsoon)

Students with B.Tech degree or M.Tech in non-relevant field requires the following two additional DC courses in this semester (3rd Semester):

Sl. No.	Course Code	Course Name	Course Type	L-T-P	Credit
1	CHC505	Advanced Process Control	DC7	3-0-0	9
2	CHC509	Computational Fluid Dynamics	DC8	3-0-0	9
				Total Credit	**18**

Course Syllabus

(a) Core Courses

D Core Course 1 **Course Code No.: CHC501** **L: T: P: 3-0-0**

Course Title : **Advanced Transport Phenomena**

Course Objectives : To provide basic unifying principles of the conservation of momentum, energy and mass with emphasis on similarities and differences amongst various transport mechanisms and to apply them to solve problems encountered in chemical engineering processes.

Learning Outcomes : Students will be able to formulate and solve differential momentum, heat, and mass balances occurring in laminar and turbulent conditions.

Modules	Topic	Lectures
1. Vector analysis	Vector and tensor operations, vector calculus, curvilinear coordinate systems.	4
2. Momentum transport	Continuum hypothesis, Newtonian and non - Newtonian fluids, diffusive and convective fluxes.	3
3. Equations of change	A short review of shell balance method.	3
	Navier-Stokes equation and their solution techniques under different boundary conditions.	3
	Similarity solution, eigen value problems and Sturm-Liouville theory.	3
4. Boundary layer theory and turbulence	Blasius exact solution method, potential flow, stream function and stream potential, turbulence phenomena.	5
5. Energy transport	Energy equation, forced and natural convection.	4
	Solution of heat flow under steady and unsteady state conditions.	6
6. Mass transport	Diffusion, application of shell balance method and equations of change for mass transfer problems.	2
	Concentration distributions for isothermal and non-isothermal mixtures. Steady and unsteady state mass transfer.	2
7. Analogy of transport	Analogy between momentum, mass and heat transfer.	4
	Total	39

Text Books:

1. Deen, W. M. (1998). *Analysis of Transport Phenomena*. Oxford Univ. Press.
2. Bird, R. B., Stewart, W. E. and Lightfoot, E. N. (2007). *Transport Phenomena*. 2nd Ed. McGraw Hill.

Reference Books:

1. Leal L.G. (2008). *Advanced Transport Phenomena: Fluid Mechanics and Convective Transport Processes*. Cambridge Univ. Press.

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<u>**D Core Course 2**</u> **Course Code No.: CHC502** **L: T: P: 3-0-0**

Course Title : **Advanced Chemical Engineering Thermodynamics**

Course Objectives : The course aims to impart advanced knowledge on chemical engineering thermodynamics, particularly phase equilibria, thermodynamics of solution and chemical equilibria including molecular thermodynamics.

Learning Outcomes : Students will be able to formulate solutions to phase and chemical equilibria problems for complex systems based on classical and molecular thermodynamics and to relate thermodynamic concepts to applications in separation and chemical reactions encountered in chemical process industries.

Modules	Topic	Lectures
1. Review of basic concept	Comparison between classical and statistical thermodynamics, equations of state.	7
2. Introduction to molecular thermodynamics	Intermolecular forces, potential function and its application in chemical engineering.	6
3. Thermodynamic properties	Intermolecular forces and the theory of corresponding states, entropy calculations, maxwell relations, equilibrium and stability, thermodynamics properties of single phase, single and multicomponent systems.	5
4. Theory of solution	Chemical potential, fugacities, activities, activity coefficients, solubility of solids/ liquids/ gases in liquids/ gases, vapour – liquid equilibria at low and high pressures, liquid – liquid equilibria, solid – vapour – liquid equilibria.	4
5. Phase equilibria	Colligative properties, phase equilibria in solutions, electrolytes, Gibbs-Duhem equation.	8
6. Reaction equilibria	Chemical equilibria, equilibrium constants for homogeneous and heterogeneous reactions, simultaneous reaction and phase equilibria .	5
7. Exergy	Exergy analysis.	4
	Total	**39**

Text Books:

1. Sandler, S.I. (2017). *Chemical, Biochemical and Engineering Thermodynamics*. 5th Ed., Wiley.
2. Smith, J. M., van Ness, H. C., and Abbott, M. M. (2004). *Introduction to Chemical Engineering Thermodynamics*. 7th Ed., McGraw–Hill.

Reference Books:

1. Prausnitz, J. M., Lichtenthaler, R. N., and de Azevedo, E. G. (1999). *Molecular Thermodynamics of Fluid–Phase Equilibria*. Prentice Hall.
2. Haile, J. M. (1992), *Molecular Dynamics Simulation: Elementary Methods*. Wiley.

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<u>D Core Course 3</u> **Course Code No.: CHC503** **L: T: P: 3-0-0**

Course Title : **Computational Techniques in Chemical Engineering**

Prerequisite : Process modelling and simulation

Course Objectives : To provide basic computational techniques in solving problems encountered in chemical engineering systems and their analysis.

Learning Outcomes : Students will have proficiency in solving chemical engineering problems using computational techniques and tools.

Modules	Topics	No of classes
1. Solution of linear algebraic equations	Error analysis, accuracy, precision, gauss elimination, Gauss-Jordan, Gauss-Seidel, LU decomposition, Cholesky decomposition and tridiagonal matrix algorithm approaches.	10
2. Solution of non-linear algebraic equations	Bisection, regula-falsi, secant, Newton- Raphson and Muller's methods.	04
3. Regression & Interpolation	Tests of significance, analysis of variance, linear and nonlinear regression analysis, Newton's forward/backward interpolation, Lagrange's interpolation and spline interpolation.	06
4. Solution of ordinary differential equations	Initial value problems: Euler's and Runge-Kutta methods, system of ODEs and adaptive Runge-Kutta methods and boundary value problems: shooting and finite difference methods.	10
5. Solution of partial differential equations	Finite differences, solutions of elliptic and parabolic types of equations.	09
	Total	39

Text Books

1. Chapra, S. C. (2009). *Numerical Methods for Engineers and Scientists*. 6th Ed., McGraw–Hill.
2. Hoffman, J. D. (2001). *Numerical Methods for Engineers and Scientists* 2nd Ed., CRC Press.

Reference books

1. Davis, M. E. (2013). *Numerical Methods and Modelling for Chemical Engineers*. Courier Corporation.
2. Constantinides, A. (1999). *Numerical Methods for Chemical Engineers with MATLAB Applications.* Prentice Hall PTR.

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<u>D Core Course 4</u> **Course Code No.: CHC504** **L: T: P: 3-0-0**

Course Title	**:**	**Advanced Chemical Reaction Engineering**
Course Objectives	**:**	To provide a comprehensive study of chemical reaction engineering including design of equipment and practical applications.
Learning Outcomes	:	The students will have knowledge of multiphase reactor design with non-isothermal, heterogeneous catalysis and catalytic reaction engineering.

Modules	Topics	Lectures
1. Non- ideality	Review of analysis of isothermal reactors and non–ideality in reactors.	4
2. Non catalytic Kinetics	Kinetics of fluid– particle non–catalytic reactions, fluid–fluid non–catalytic reactions and application to design.	9
3. Heterogeneous reactions	Diffusion and reaction: External diffusion effects on heterogeneous reaction, diffusion and reaction in spherical pellets, internal effectiveness factor, estimation of diffusion and reaction limited regimes, Wisz-Prater criterion for internal diffusion, Mears criterion for external diffusion, inter pellet heat and mass transfer.	9
4. Solid catalysis	Introduction, definitions, catalytic properties, classification of catalysts, steps in catalytic reaction, adsorption isotherm, chemisorption's, synthesizing rate law, mechanism and rate limiting steps, deducing a rate law from the experimental data, finding a mechanism consistent with experimental observation, evaluation of rate law parameters, catalyst promoters and inhibitors, catalyst deactivation.	9
5. Catalyst characterization	Catalyst synthesis: impregnation and other techniques, physico-chemical characterization of catalyst.	8
	Total	39

Text Books:

1. Fogler, H. S. (2008). *Elements of Chemical Reaction Engineering*. 4th Ed., Prentice Hall.
2. Levenspiel, O. (2006). *Chemical Reaction Engineering*. 3rd Ed., Wiley.

Reference Books:

1. Carberry, J. J. (2001), *Chemical and Catalytic Reaction Engineering*. McGraw–Hill.
2. Froment, G. F., Bischoff, K. B., and De Wilde, J. (1979). *Chemical Reactor Analysis and Design*. Wiley.
3. Smith, J. M. (1981). *Chemical Engineering Kinetics*, McGraw–Hill. 3rd Edition.

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<u>D Core Course 5</u> **Course Code No.: CHC505** **L: T: P: 3-0-0**

Course Title : **Advanced Process Control**

Course Objectives : To provide theoretical background with detailed mathematical analysis of dynamic behaviour of chemical process systems and to emphasize process control techniques that are used in practice, including stability analysis and design of control systems.

Learning Outcomes : Students will have basic and advanced control strategies and algorithms and shall be able to design control systems needed for chemical processes.

Modules	Name of the Topic	Lectures
1. Introduction	Introduction, modelling of dynamic behaviour of chemical processes, transfer function and state–space representation.	05
	Dynamic analysis of chemical processes, frequency response analysis	07
2. Design of controllers and tuning techniques	Design of conventional controller, performance criteria, controller tuning, Ziegler-Nichols tuning, empirical methods of tuning.	04
3. Stability analysis	Stability analysis in transfer function and state–space domain.	08
4. Advanced control system	Analysis and design of complex control schemes – cascade control, feedforward control, split-range control, ratio control and inferential control	06
5. MIMO	Synthesis and analysis of MIMO control processes, interaction of control loops, relative gain array and the selection of loops, and decoupling strategies.	05
6. Model based control	Model predictive control and its implementation.	04
	Total	**39**

Text Books:

1. Stephanopoulos, G. (2008). *Chemical Process Control: An Introduction to Theory and Practice*. 3rd Ed. Prentice Hall.
2. Seborg, D. E., Mellichamp, D. A., Edgar, T. F., and Doyle, F. J. (2009). *Process Dynamics and Control*. 2nd Ed., John Wiley & Sons.

Reference Books:

1. Ogunnaike, B. A., and Ray, W. H. (1994). Process *Dynamics, Modeling and Control*. Oxford University Press.
2. Bequette, B. W. (2013). *Process Control: Modeling, Design and Simulation*, Prentice Hall India

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D Core Course 6 **Course Code No.: CHC508** **L: T: P: 3-0-0**

Course Title : **Advanced Mass Transfer**

Course Objectives : To extend the fundamental concepts of mass transfer in cases of multicomponent systems (with and without chemical reactions) and the application of those concepts in solving real engineering problems.

Learning Outcomes : Students shall have adequate knowledge in tackling engineering problems with complex mass transfer operations.

Modules	Name of the Topic	Lectures
1. Review	VLE and VLLE of binary system, Introduction to Multi-phase equilibrium, ternary diagram, residual curve, ideal solution of multi-components	3
2. Thermodynamic correlation	Multi-phase equilibrium, K-value and activity coefficient	3
3. Multi-component diffusion and convection	Multi-component diffusion, convective mass transfer, correlations for mass transfer coefficients, review of the models for mass transfer at fluid–fluid interface.	4
4. MESH equations	Formulation of Material and Energy balance equation (MESH) for single stage operation, batch distillation, flash vaporization, degrees of freedom (DOF)	4
5. Short-cut methods	Short-cut methods for designing multi-component multi-stage fractionation: Kremser equation, Fenske–Underwood–Gilliland, Wang–Henke, Naphtali–Sandholm, Thiele–Geddes	3
6. Rigorous methods	Rigorous method of multi-component multi-stage fractionation: MESH Equations for multi-stage fractionation, DOF, Solution technique	6
7. Multicomponent distillation	Multi-component distillation and cascading of columns, divided-wall distillation columns	4
8. Reactive mass transfer	Introduction to reactive distillation (RD) process, advantages and disadvantages of RD, design of RD columns. Mass transfer: Gas liquid reactions: solutions for slow, fast and instantaneous reactions with adsorption for single and two gases.	9
9. Supercritical Fluid Extraction	Supercritical fluid extraction	3
	Total	39

Reference Books:

1. Seader, J. D., Henley, E. J., & Roper, D. K. (1998). *Separation Process Principles*. John Wiley & Sons.
2. Taylor, R., & Krishna, R. (1993). *Multicomponent mass transfer*. John Wiley & Sons.
3. Doraiswamy, L.K. & Sharma, M.M (1984) Heterogeneous reaction: analysis, examples and reactor design vol2 , Fluid-fluid Solid reaction, Wiley.
4. Kulprathipanja, S. (2002). *Reactive separation processes*. Taylor & Francis: New York.

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D Core Course 7 **Course Code No.: CHC509** **L: T: P: 3-0-0**

Course Title : **Computational Fluid Dynamics**

Course Objectives : To provide basic theoretical understanding to the students on mathematical formulation and different approaches underlying computational techniques in fluid flow, heat and mass transfer.

Learning Outcomes : Students will have sufficient knowledge to formulate and solve various problems using CFD including CFD tools.

Modules	Name of the Topic	Lectures
2. Introduction to CFD	Basics of CFD and its importance.	3
3. Basic Conservation Laws	Reynold transport theorem: Integral and Differential forms of Conservative equation: Continuity Equation, Navier Stokes equation, energy equation.	4
4. PDE characteristics	Classification of PDES: linear, non-linear characteristics equation, parabolic, elliptic and hyperbolic equations, examples of such equations in fluid mechanics and heat Transfer.	3
5. Weighted residual Method	Discretization methods, finite volume method.	2
6. Steady diffusion	Discretization internal and boundary grid points and, Interface conductivity, source term Linearization.	7
7. Unsteady diffusion	Explicit, implicit, discretization for unsteady for 2D and 3D.	3
8. Solution methods	Linear algebra, direct method, TDMA, line by line, iterative Gauss Seidel, point wise, diagonal dominance, concept of convergence (Graphical) and relaxation parameter.	3
9. Advection diffusion	Upwind, Peclet number, exponential and hybrid scheme, numerical diffusion.	5
10. Flow solution	Staggered grid solution algorithm for Pressure-Velocity coupling: SIMPLE,SIMPLER	6
11. Turbulence modelling	Review of turbulence, direct numerical simulation (DNS), large eddy simulation (LES), and two-equation model.	3
	Total	39

Text Books:
1. Versteeg, H.K. & Malalasekera, W. (1995) *Introduction to Computational Fluid Dynamics: The Finite Volume Method* John Wiley & Sons Inc.
2. Patankar, S. (1980) *Numerical heat transfer and fluid flow*, Taylor & Francis.

Reference Books:
1. Chung, T. J. (2002) *Computational Fluid Dynamics*, Cambridge Univ. Press.

(b) Elective Courses

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D Elective Course 1 **Course Code No.:** CHE501 **L: T: P: 3-0-0**

Course Title	:	**Membrane Technology**
Prerequisite	:	Mass Transfer, Fluid Mechanics.
Course Objectives	:	To provide an in-depth knowledge i) in membrane separation processes and ii) on the selection of a membrane process for different applications and iii) operational issues, limitations and system configuration, and design.
Learning Outcomes	:	Students will be able to i) characterize membrane and calculate membrane flux, permeability etc. ii) solve problems for any application in chemical processes, biotechnology, environmental pollution control etc., and iii) clean and wash membranes for their reutilization.

Modules	Name of the Topic	Lectures
1. Overview of membrane science and technology	Types of Membranes, Membrane Processes- microfiltration, ultrafiltration, nanofiltration, and reverse osmosis.	5
2. Membrane transport theory	Solution-diffusion model, pore-flow membranes.	3
3. Membranes and modules	Isotropic membranes, anisotropic membranes, inorganic membranes, liquid membranes and hollow fiber membranes.	9
4. Concentration polarization and fouling	Concentration polarization in liquid separation processes, gel layer model, osmotic pressure model, boundary layer resistance model, concentration polarization in gas separation processes, membrane fouling and fouling control.	10
5. Applications of membrane processes and economics	Gas separation, pervaporation, ion exchange membrane processes, membrane contactors, membrane distillation, membrane reactors and membrane bioreactors, medical applications of membranes, membranes for water treatment and desalination	10
6. Economic analysis	Economic analysis of membrane processes	2
	Total	39

Textbooks:

1. Baker, R. W. (2012), *Membrane Technology and Applications*, 3rd Ed., Wiley, UK.
2. Mulder, M. Mulder, J. (1996) "*Basic Principles of Membrane Technology*", Kluwer Academic.

Reference books:

1. W. S. W. Ho and K. K. Sirkar (1992), *Membrane Handbook*, Chapman & Hall, NY.
2. N.N. Li, A. G. Fane, W.S.W. Ho and T. Matsuura, (2008), *Advanced Membrane Technology*, Wiley.
3. M. Cheryan, (1998), *Ultrafiltration and Microfiltration Handbook*, CRC Press.

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D Elective Course 2 **Course Code No.: CHE502** **L: T: P: 3-0-0**

Course Title : **Nanotechnology**

Prerequisite : Thermodynamics and Transport Phenomena

Course Objectives : To address the fundamental concepts of nanotechnology, synthesis and characterization techniques for nanomaterials.

Learning Outcomes : Students will have an insight into the area of nanotechnology and its application in chemical engineering problems.

Modules	Name of the Topic	Lectures
1. **Introduction to nanotechnology**	History, definitions, particle size, chemistry and physics of nanomaterials, safety issues with nanoscale powders.	6
2. **Preparation of nanomaterials**	Top down and bottom up approach, synthesis of different nanomaterials. theory of nucleation and growth.	9
3. **Characterization of nanoparticles**	Scanning probe microscopes (atomic force microscopy, scanning tunnelling microscopy), transmission electron microscopy, scanning electron microscopy.	9
4. **Nanocomposites**	Nanofillers, high performance materials, polymer nanocomposites, nanoclays, nanowires, nanotubes, nanoclusters.	9
5. **Nanomaterials application**	Application of nanoparticles and nanomaterials in different fields of chemical engineering, biotechnology, sensors, etc.	6
	Total	**39**

Text books:

1. Kulkarni, S. K. (2007). *Nanotechnology Principles and Practices*, Capital Publishing.
2. Rogers, B. Pennathur, S. Adams, J. (2008). *Nanotechnology: Understanding small systems*, Taylor and Francis.
3. Ajayan, P. M. Schadler, L. S. and Braun, P. V. (2004) *Nanocomposite Science and Technology*, Wiley.

Reference books:

1. Regis, E. (1995) *Nano: The Emerging Science of Nanotechnology*, Back Bay Books.
2. Cao, G. and Wang, Y. (2004) Nanostructures and Nanomaterials: Synthesis, Properties, and Applications, World Scientific.

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<u>**D Elective Course 3**</u> **Course Code No:** CHE503 **L: T: P: 3-0-0**

Course Title : **Catalysts and materials characterization techniques**

Course Objectives : To provide knowledge on basic and advanced characterization techniques for catalysts and other materials used in chemical processes.

Learning Outcomes : Students will have essential knowledge on characterization techniques for catalysts and other materials.

Module	Topics	Lectures
1. Structural analysis	Surface area and pore analysis using different techniques like BET, BJH, mercury porosimetry, etc.X-ray diffraction (XRD) for characterization of bulk crystal structure and chemical phase composition,X-ray photoelectron spectroscopy (XPS) for surface characterization	10
2. Chemisorption technique	Determination of metal dispersion on catalyst surface and metal area using hydrogen and carbon monoxide chemisorption studies.	4
3. Thermal analysis	Temperature programmed reduction (TPR) for rate of reduction of active metals, Effect of temperature and correlations with catalyst activity.	7
	Rate of desorption using temperature programmed desorption (TPD) for adsorbed molecules as a function of temperature and acid – base properties of catalysts.	2
	Use of thermo gravimetric analysis (TGA) in the analysis of thermal-mass-loss and energy analysis	2
4. Spectroscopic techniques	UV-vis, Infra-red and Raman spectroscopy for concentration measurement, interaction of metal oxides, band gap, etc, identification of compounds and oxidation state.	7
5. Microscopic techniques	Scanning electron microscopy (SEM) for imaging topography of solid surface Transmission electron microscopy (TEM) for determination of the micro – texture and micro structure	7
	Total	39

Reference Books:

1. Carberry, J.J. (2001). *Chemical and catalytic reaction Engineering*, Dover Publications.
2. Leng, Y. (2008). *Materials Characterization: Introduction to microscopic and spectroscopic methods*. Wiley.
3. Kaufmann (Ed), E.N. (2003). *Characterization of Materials*, Wiley –Inter Science.
4. Ertl, G. Knozinger, H. and Weitkamp, J. (1997). *Handbook of Heterogeneous Catalysis*, Vol. 2, Wiley VCH.
5. Banwell, Colin N. & McCash, Elaine M. (2000). *Fundamentals of Molecular Spectroscopy*. Tata McGraw-Hill Pub. Co.

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<u>**D Elective Course 4**</u> **Course Code No.:** CHE504 **L: T: P: 3-0-0**

Course Title : **Process Optimization**

Course Objectives : To provide basic knowledge about optimization of processes and plants using various linear and non-linear techniques.

Learning Outcomes : Students will be able to**:** i) formulate optimization problems**,** ii) recognize various decision variables, and iii) solve optimization problems using classical and advanced optimization algorithms.

Modules	Name of the Topic	Lectures
1. Introduction to process optimization	Formulation of various process optimization problems and their classification, basic concepts of optimization-convex and concave functions, necessary and sufficient conditions for stationary points.	5
2. Optimization of unconstrained functions (One dimensional search)	Optimization of one-dimensional functions, bracketing methods: exhaustive search method, bounding phase method, interval halving method, Fibonacci search method, golden section search method, Newton-Raphson method, secant method.	5
3. Unconstrained multivariable optimization	Direct methods: random search, grid search, univariate search, simplex method, conjugate search directions, Powell's method, indirect methods- gradient and conjugate gradient method, Newton's and Quasi-Newton method.	9
4. Linear programming and applications	Basic concepts in linear programming, the simplex method of solving linear programming problems, standard LP form, obtaining a first feasible solution, LP applications.	4
5. Nonlinear programming with constraints	The Lagrange multiplier method, necessary and sufficient conditions for a local minimum; quadratic programming, generalized reduced gradient method, penalty function and augmented Lagrangian methods; successive quadratic programming, NLP applications.	10
6. Mixed integer programming	MILP, branch and bound technique, MINLP, outer approximation methods, applications.	2
7. Genetic algorithms	Working principles, differences between GAs and traditional methods; similarities between GAs and traditional methods, GAs for constrained optimization, other GA operators, real coded GAs, multi-objective GAs, applications.	4
	Total	**39**

Textbooks:

1. Edgar, T.F. Himmelblau, D.M. (2001) *Optimization of Chemical Processes*, McGraw-Hill.
2. Rao, S.S. (1996) *Engineering Optimization: Theory and Practice*, Wiley.
3. Dutta, S. (2016) *Optimization in Chemical Engineering,* 1st Ed., Cambridge Univ. Press.

Reference books:

1. Fletcher, R. (2013) *Practical Methods of Optimization*, Wiley.
2. Floudas, C. A. (1995) *Nonlinear and Mixed-Integer Optimization: Fundamentals and Applications*, Oxford Univ. Press.

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D Elective Course 5 **Course Code No.:** CHE505 **L: T: P: 3-0-0**

Course Title : **Interfacial and Colloidal Phenomena**

Course Objectives : To impart knowledge on fundamentals of interfacial and colloidal phenomena and colloidal interactions between surfaces, particles and surfactants.

Learning Outcomes : Students will gain insight into interfacial and colloidal phenomena and will be able to solve problems encountered in chemical engineering systems.

Modules	Name of the Topic	Lectures
1. **Introduction**	Introduction to colloids, interfaces, surfactants and emulsions, micelle formation.	5
2. **Interaction forces**	Intermolecular forces, van der Waals forces (Keesom, Debye, and London interactions), colloidal systems and colloidal stability (van der Waals attraction and potential energy curves), Brownian motion and flocculation.	8
3. **Surface tension**	Surface and interfacial tension, surface free energy, surface tension for curved interfaces, surface excess and Gibbs equation, theory of surface tension and contact angle and wetting.	8
4. **Thermodynamics**	Thermodynamics of interfaces, micelles and mixed micellar formations.	5
5. **Electrokinetic phenomena**	Electrical phenomena at interfaces, electrical double layer.	5
6. **Advanced materials**	Advanced and functional interfaces – superhydrophobicity, functional coatings, structural colors, nano– adhesives, nanocomposites.	8
	Total	**39**

Text books:

1. Hiemenz, P. C., and Rajagopalan, R. (1997), *Principles of Colloid and Surface Chemistry*, Marcel Dekker.
2. Myers, D. (1991), *Surfaces, Interfaces, and Colloids: Principles and Applications*, Wiley.

Reference books:

1. Masliyah, J. H. and Bhattacharjee S. (2005), *Electrokinetic and Colloid Transport Phenomena*, Wiley.
2. Rosen, M. J. (2004), *Surfactants and Interfacial Phenomena*, Wiley-Interscience.

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D Elective Course 6 **Course Code No.: CHE506** **L: T: P: 3-0-0**

Course Title : **Carbon Capture and Clean Energy**

Course Objectives : To acquire underlying principles of science and engineering of CO_2 capture from vents and exhausts of various processes and to provide a blue print for minimising carbon footprint through the usage of technology e.g. power cycles, heat recovery and heat utilization.

Learning Outcomes : Students will have enough knowledge about CCS and various climate change mitigation technologies.

Modules	Topics	Lectures
1. Introduction to fossil fuels & carbon emission	World energy scenario, fossil fuel and emissions, importance of power plants and other processes of carbon emissions e.g., lime and cement manufacture, natural and synthesis gas processing plants, etc.	08
2. Combustion and gasification technologies	Post combustion treatment technologies, supercritical processes, fluidized beds, IGCC, oxyfuel gasification and combustion and clean-up processes, syngas from different energy sources, e.g. fossil fuels, biomass, gas reforming, partial oxidation and other routes to syngas/hydrogen production, routes to alternative liquid fuels – synthetic and bio-diesel, DME, GTL, polygeneration.	12
3. Carbon capture	Technology options for CO_2 capture, advantages and disadvantages of major CO_2 capture technologies, global issues and trends.	06
4. Carbon storage & sequestration	Storage options, technologies and field projects, carbon sequestration methods	07
5. Highly efficient power generation	Utilization and recovery of low grade and waste heat, combined heat and power cycle, the emerging technologies.	06
	Total	**39**

Reference Books:

1. Rackley, S. A. (2017). *Cabon Capture and Storage*. 2nd Ed. Butterworth-Heinemann.
2. Herzog, H.J. (2018) *Carbon Capture*, MIT Press.
3. Kohl, A. L.; Nielsen, R. B. (1997) *Gas Purification*, 5th Ed., Gulf Publishing.
4. Higman, C. and Buggt, M. (2008) *Gasification*, 2nd ed., Gulf Professional Publishing.
5. Liu, K. Song, C. Subramani, V. (2010) *Hydrogen and Syngas Production and Purification Technologies*, AIChE, Wiley.

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D Elective Course 7 **Course Code No.:** CHE507 **L: T: P: 3-0-0**

Course Title : **Modelling & Simulation**

Prerequisite : UG Courses on Mathematics, Computer Programming, Chemical Engineering Thermodynamics, Heat and Mass Transfer.

Course Objectives : To apply the concepts of chemical engineering in formulating complex engineering problems, suitable techniques to solve them and validation of simulation results.

Learning Outcomes : Students shall be able to analyze and design complex processes using their own computer code and use of available computational tools.

Modules	Topics	Lectures
1. Basic concepts of process modelling	Advantages and limitations of process models; continuum and discrete domain, classification of models–phenomenological, stochastic and empirical, lumped and distributed parameters, Population Balance models; Monte Carlo Simulation. Properties of materials and their estimation.	7
2. Tools and techniques of simulation	CFD and flow-sheet simulation tools, multi-scale and multi-physics modelling techniques, AI based models – ANN, Fuzzy and hybrid.	5
3. Steady–state modelling	Development of steady-state mathematical model of process equipment's in heat transfer, mass transfer, and reaction engineering such as steady state models of flash vaporizer, distillation column, absorbers, CSTR.	10
4. Simulation	Review of solution procedures and available numerical libraries, solution of simultaneous nonlinear algebraic and transcendental models equations.	6
5. Flow sheeting	Introduction to steady-state flow-sheeting, approaches to flow-sheeting systems, introduction to available commercial process simulators.	5
6. Unsteady Problems	Unsteady-state initial value and boundary value problems; Eigen value problems.	4
7. Error Analysis	Error estimation and reconciliation.	2
	Total	39

Text Books:

1. Rasmuson, A., Andersson, B., Olsson, L., & Andersson, R. (2014). *Mathematical modeling in chemical engineering*. Cambridge University Press.
2. Luyben, W. L. (1989). *Process modeling, simulation and control for chemical engineers*. McGraw-Hill Higher Education.Upreti, S. R. (2017). *Process Modeling and Simulation for Chemical Engineers: Theory and Practice*. John Wiley & Sons.

Reference Books:

1. Constantinides, A., Schowalter, W. P., Carberry, J. J., & Fair, J. R. (1987). *Applied numerical methods with personal computers*. McGraw-Hill, Inc.
2. Seader, J. D., Henley, E. J., & Roper, D. K. (1998). *Separation Process Principles*. John Wiley & Sons.
3. Poling, B. E., Prausnitz, J. M., & O'connell, J. P. (2001). *The properties of gases and liquids* (5 e/d). New York: Mcgraw-hill.
4. Bequette, B. W. (2003). *Process control: modeling, design, and simulation*. Prentice Hall Professional.

(c) Open electives

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Open Elective Course 1 **Course Code No.: CHO501** **L: T: P: 3-0-0**

Course Title : **Rheology**

Course Objectives : To impart knowledge on the fundamental concepts of rheology, methods of determination of rheological characteristics and the analysis of various rheological problems, encountered in engineering applications.

Learning Outcomes : The students will have adequate knowledge of rheology of fluids and complex fluids/mixtures, the significance of various rheological parameters and their usage in engineering.

Modules	Topics	Lectures
1. Introduction to rheology	Rheology of fluids and complex mixtures- macromolecules solutions, melts, gels etc., multiphase systems- dispersions, emulsions and gels. microscopic mechanisms: interactions unusual flow phenomena.	06
2. Mathematical concepts	Tensors, index notation, operations with tensors, kinematics-deformation measures, balances of mass and momentum, frame invariance.	05
3. Rheometry	Stress, strain, velocity gradient, strain rate, viscometric flows- shear flow, extensional flow, types of rheometers and their operational features, rheometric measurements: material functions: viscosity, creep compliance, relaxation modulus, storage and loss moduli, tan δ, normal stresses and experimental observations.	11
4. Macroscopic continuum Models	Simplistic Models**-** Viscous fluids: Newtonian, generalized Newtonian, viscoelastic materials: Maxwell, Jeffreys, governing equations, constitutive relations, linear viscoelastic materials, time-temperature superposition, relaxation time spectrum, non-linear models: convected derivatives non-linear viscoelastic measurements	11
5. Microscopic models	Microscopic origin of stress, elastic dumbbell model, overview of other models- Rouse, Zimm, Doi-Edwards (reptation)	06
	Total	39

Text Books:

1. Bird, R.B., Armstrong, R.C. and Hassager, O.J. (1987). *Dynamics of Polymeric Liquids*. Wiley.

Reference Books:

1. Larson, R.G. (1999). *The Structure and Rheology of Complex Fluids*. Oxford Univ. Press.

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Open Elective Course 8 **Course Code No.:** CHE502 **L: T: P: 3-0-0**

Course Title : **Fluidization Engineering**

Prerequisite : Fluid Mechanics, Heat & Mass Transfer

Course Objectives : The objective of the course is to introduce the developments in the field of fluidization engineering that are pertinent to the engineers and potential users of fluidized beds.

Learning Outcomes : Understanding of the basic phenomenon of fluidization and the design of fluidized bed systems for various industrial applications.

Modules	Topics	Lectures
1. Introduction	Phenomenon of fluidization, comparison with other contacting methods, industrial applications of fluidization, advantages and disadvantages of fluidized beds, industrial applications.	08
2. Fundamentals of fluidization	Characterization of bed particles, regime of operations in gas-solid contacting, fluidization without carryover of particles, types of gas fluidization without carryover, the Geldart classification of particles, fluidization with carryover of particles, types of gas fluidization with carryover, mapping of fluidization regimes.	08
3. Contacting regimes	Gas-solid interaction in the gas entry region of the bed, types and design of distributors, power consumption, gas-solid interaction in the bubbling bed - bubbles in dense beds, bubbling beds, the lean zone above the dense bed, behaviour of single rising bubble, estimation of bed properties, physical and flow models for bubbling fluidization bed, freeboard behaviour, entrainment and elutriation, estimation of TDH, gas dispersion and interchange in bubbling bed, applications.	13
4. High-velocity fluidization	Turbulent fluidized beds, fast fluidization, freeboard-entrainment model applied to fast fluidization, pressure drop in turbulent and fast fluidization, mixing and movement of solids, applications.	07
5. Design and application	General design of a fluidized bed, case study of a process involving fluidized bed (e.g. FCC).	03
	Total	**39**

Text Book:

1. Kunii, D. Levenspiel, O. (1991) *Fluidization engineering*, 2nd Ed. Butterworth—Heinemann.

Reference Books:

1. Davidson, J.F. Clift, R. and Harrison, D. (1985) *Fluidization*, 2nd Ed., Academic Press, London.
2. Leva, M. (1959) *Fluidization*, McGraw-Hill, New York.

(d) Labs

Departmental Practical **Course Code No.:** CHC506 **L: T: P: 0-0-3**

Course Title : Instrumental Methods of Analysis

Course Objectives : To expose the students to different analytical equipment/instruments that are useful for carrying out research in different areas in chemical engineering.

Learning Outcomes : Students will be proficient in using instrumental techniques in chemical engineering.

Units	**Name of the experiment**
1. Analytical instruments/equipment	Studies on **UV-vis spectrometry.**
	Particle size distribution measurements using **Zeta Sizer.**
	Particle size distribution measurements using **Particle size Analyzer.**
	Detection of functional groups using **FTIR** Analysis.
	Size reduction studies using **Planetary ball mill**
2. Flow characterization & wettability	Rheometric analysis of fluids using **Rheometer.**
	Contact angle measurements techniques using **Goniometer.**
3. Optical instruments	Surface characterization using **Optical Microscopy.**
	Refractive index measurement using **Refractometer.**
4. Elemental analysis	Ultimate analysis of solid fuel using **CHNS analyzer.**

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Departmental Practical **Course Code No.:** CHC507 **L: T: P: 0-0-3**

Course Title : Computational Techniques Lab

Course Objectives : To expose the students to computational techniques required for design in chemical engineering and solution of problems.

Learning Outcomes : Proficiency in using computational techniques to solve problems in chemical engineering.

S. No.	Name of the experiment	classes
1.	Developing a computer codes for the numerical solution of system of simultaneous linear algebraic equations : a) Gauss elimination method b) Gauss Seidel iterative method	02
2.	Developing a computer program for the numerical solution of single and multivariable non-linear algebraic equation using: a) Bisection method b) Newton-Raphson method	02
3.	Linear and non-linear regression for chemical engineering data	02
4.	Developing a computer program to perform interpolation	01
5.	Developing a computer program for the numerical solution of a set of ordinary differential equations using a) 4^{th} order Runge-Kutta method b) predictor-corrector	02
6.	Developing a computer program for the numerical solution of partial differential equations: Liebmann method	01

Departmental Practical **Course Code No.:** CHC510 **L: T: P: 0-0-3**

Course Title : Advanced Chemical Engineering Lab

Course Objectives : To make the students conversant of CFD and flow sheet simulation techniques.

Learning Outcomes : Students will be proficient in conducting simulations using advanced simulation tools.
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S. No.	Name of the experiment	classes
CFD simulation	CFD simulation for flow and heat transfer	05
Process simulation	Flowsheet simulation using Aspen Plus	05