Indian Institute of Technology Kanpur

COURSES OF STUDY

2026





Indian Institute of Technology Kanpur
KANPUR-208016

CHEMICAL ENGINEERING

Template for the BT program in Chemical Engineering

Semester 1	Semester 2	Semester 3	Semester 4	Semester 5	Semester 6	Semester 7	Semester 8

SCHEME-1 (9) ELC111/ELC112/ ELC113 *	ETH111 (3) **	SCHEME-2 HSS-I (9-11)	SCHEME-3 EME (9-11)	SCHEME-4 HSS-II (9)	SCHEME-5 HSS-II (9)	SCHEME-6 HSS-II (9)	
MTH 111 (6)	MTH 113 (6)	ESC201 (14)	CHE212 (12)	CHE311 (12)	CHE352 (12)	CHE453 (6)	
MTH 112 (6)	MTH 114 (6)	ESO201 (11)	CHE213 (12)	CHE331 (12)	CHE655 (12) /CHE668 (9)		
PHY 112 (11)	PHY 113 (11)	ESO204 (11)	CHE221 (12)	CHE381 (12)	DE-2 (9)	DE-3 (9)	OE-4 (9)
PHY 111 (3)	CHM 111 (3)	CHE201 (3)	CHE261 (9)	DE-1 (9)	OE-1 (9)	OE-2 (9)	OE-5 (9)
TA 111 (9)	ESC 111 (7)	CHE251 (12)	CHE200 (2)			OE-3 (9)	OE-6 (9)
CHM 112 (4)	ESC 113 (7)						
CHM 113 (4)	LIF111 (6)						
PE111 (3)	PE112 (3)						
55	52	60-62	56-58	54	48-51	42	27
27 credits of DEs and 54 credits of OEs to be taken in the 5th to 8th semester.							

Credit table for BT program in Chemical Engineering		
Course type	Recommended Credit	Credit in the department
Institute Core (IC)	112	112
E/SO	18-45	22
Department	144-179	152-155 (125-128 DC + 27 DE)
Open electives (OE)	51-57	54
SCHEME	54-58	54-58
Total for 4-year BT/BS	391-420	394-401

Template for the BTH program in Chemical Engineering

Template for 3rd to 8th semester for BTH program in Chemical Engineering					
Semester 3	Semester 4	Semester 5	Semester 6	Semester 7	Semester 8
SCHEME-2 HSS-I (9-11)	SCHEME-3 EME (9-11)	SCHEME-4 HSS-II (9)	SCHEME-5 HSS-II (9)	SCHEME-6 HSS-II (9)	
ESC201 (14)	CHE212 (12)	CHE311 (12)	CHE352 (12)	CHE453 (6)	
ESO201 (11)	CHE213 (12)	CHE331 (12)	CHE655 (12) /CHE668 (9)	UGP-2 (9)	OE-4 (9)
ESO204 (11)	CHE221 (12)	CHE381 (12)	UGP-1 (9)	OE-2 (9)	OE-5 (9)
CHE201 (3)	CHE261 (9)	DE-1 (9)	OE-1 (9)	OE-3 (9)	OE-6 (9)
CHE251 (12)	CHE200 (2)		DEH-1 (9)	DEH-2 (9)	DEH-3 (9)
60-62	56-58	54	57-60	51	36
2 UGPS, (UGP-1 and UGP-2 in lieu of two DEs in the BT template), 9 credits of DE, 27 credits at 6/7 level as DEH and 54 credits of OEs to be taken in the 5th to 8th semester.					

— CPI criteria for BTH: 8.0

Template for the BTM program in Chemical Engineering

Template for 3rd to 8th semester for BTM program in Chemical Engineering					
Semester 3	Semester 4	Semester 5	Semester 6	Semester 7	Semester 8
SCHEME-2 HSS-I (9-11)	SCHEME-3 EME (9-11)	SCHEME-4 HSS-II (9)	SCHEME-5 HSS-II (9)	SCHEME-6 HSS-II (9)	
ESC201 (14)	CHE212 (12)	CHE311 (12)	CHE352 (12)	CHE453 (6)	
ESO201 (11)	CHE213 (12)	CHE331 (12)	CHE655 (12) /CHE668 (9)		

ESO204 (11)	CHE221 (12)	CHE381 (12)	OE-2 (9)	MTB-1 (9)	MTB-4 (9)
CHE201 (3)	CHE261 (9)	OE-1 (9)	OE-3 (9)	MTB-2 (9)	MTB-5 (9)
CHE251 (12)	CHE200 (2)			MTB-3 (9)	MTB-6 (9)
60-62	56-58	54	48-51	42	27
27 OE credits and 54 MTB credits in the 5^{th} to 8^{th} semester.					

Template for five year dual-degree program in Chemical Engineering

Template for dual degree program in Chemical Engineering (Category A)					
Sem I-VI	Sem VII	Sem VIII	Summer	Sem IX	Sem X
Same as BT Template	CHE453 (6)		CHE699 (9)	CHE699 (36)	CHE699 (36)
	Complete 54 CHE PG course credits using OE/DE slots. Must do any 2 of CHE611, CHE621, CHE631 and CHE641 in the 54 CHE PG course credits				
PG Credits Summary- Thesis: 81; CHE PG Courses: 54 9 credit of DE and 36 credits of OE may be waived off in the UG requirement					

Template for dual degree program in Chemical Engineering (Category B)						
UG Pre-requisites		Sem VII	Sem VIII	Summer	Sem IX	Sem X
Odd Sem	Even Sem	CHE453 (6)		CHE699 (9)	CHE699 (36)	CHE699 (36)
ESO204/ CHE311	ESO201/ CHE221 CHE331	Complete 54 CHE PG course credits using OE/DE slots. Must do CHE611, CHE621 and CHE631/CHE633 (any one) in the 54 ChE PG				
PG Credits Summary- Thesis: 81; CHE PG Courses: 54 36 credits of OE may be waived off in the UG requirement UG Pre-requisite course is mandatory for the completion of DD-B						

Template for double major: second major in Chemical Engineering

Odd Sem	Even SEM
Pre-requisites	
ESO201 (11)	
Mandatory CHE courses	
CHE251 (12)	CHE212 (12)
CHE311 (12)	CHE213 (12)
CHE331 (12)	CHE221 (12)
CHE381 (12)	CHE352 (12)
Total CHE course credits: 96	

36 credits of OE may be waived off in the UG requirement
Pre-requisite course is mandatory for the completion of DM

Minor in Chemical Engineering

Students should complete any three of the following courses:

CHE251, CHE212, CHE213*, CHE221*, CHE311, CHE331*, CHE381

Offered in minor slots

DEPARTMENT OF ChE			
Courses ID	**Course Title**	**Credits L-T-P-D-[C]**	**Content**
ChE200	CHEMICAL ENGINEERING COMMUNICATION SKILLS	0-0-2-0-2	Introduction, listening skills, paper writing, literature search, resume and CV writing, oral presentation and public speaking, group discussion.
ChE201	INTRODUCTION TO CHEMICAL ENGINEERING	0-0-2-0-2	Introduction to Chemical Engineering Profession, Safety aspects in different Chemical Industries,Data Analysis and Fitting, Instrumentation: To measure different parameters such as pressure, temperature, velocity, flow rates, etc.,Heat Transfer: Different types of heat exchangers, evaporation units, etc...,Mass Transfer: Gas-liquid contacting devices, tray towers, adsorption, liquid-liquid contacting devices, humidification crystallization.Chemical Reaction Engineering: Reactor types such as batch, semi-batch, CSTR, plug

			flow, packed bed, fluidized bed, catalysis.Fluid-Solid separation: Different types of pumps, pipes, valves, filtration units. **Course Reference**: 1. Pushpavanam, S., Introduction to Chemical Engineering, PHI Learning Private Limited, New Delhi, 2012. 2. Morton Denn, Chemical Engineering: An Introduction, Cambridge University Press, 2011 3. Perry's Chemical Engineers' HandBook, The McGraw-Hill Companies, Inc., 2008.
ChE212	HEAT TRANSFER	3-0-3-0-12	Modes of heat transfer (Conduction, convection, radiation), Boiling, Condensation, Heat Exchanger Design, Evaporators, Heat Transfer Unit Operations, Numerical Modeling. **Course Reference:** 1. Frank P. Incropera, David P. Dewitt, Theodore L. Bergman, and Adrienne S. Lavine, Incr-opera's Principles of Heat and Mass Transfer, Wiley India ed. Wiley India. 2.J. P. Holman and Souvik Bhattacharyya, Heat Transfer, McGraw Hill; 10th ed, McGraw Hill Education. 3. Adrian Bejan, Heat Transfer, Wiley India Pvt Ltd. 4. Yunus A. Cengel and A. J. Ghajar, Heat and Mass Transfer: Fundamentals and Applications, 5th Ed. SIE, McGraw Hill Education. 5. Warren L. McCabe, Julian C. Smith and Peter Harriott, Unit Operations of Chemical Engineering, 7th ed. (Indian Ed.), McGraw Hill Education. 6. Donald Q. Kern, Process Heat Transfer, McGraw Hill, New York.
ChE213	MASS TRANSFER AND SEPARATION PROCESSES	3-0-3-0-12	Mass transfer related unit operations in process industries; Fundamental of Mass Transfer: continuous and equilibrium stage contactors; Absorption: equilibrium and rate based approach, NTU and HTU, hydrodynamic considerations; Distillation: vapor-liquid equilibrium, Ponchon-Savarit and McCabe-Thiele methods for equilibrium stage calculations, Extraction: single- and multi-stage cross-current extraction, continuous countercurrent multistage extraction; Adsorption and chromatography: single- and multistage cross-current operations, packed-bed continuous contactor; Humidification and Drying: dry and wet bulb temperatures, humidity, relative and percentage humidity, psychometry chart, and adiabatic saturation temperature; mechanisms of batch drying, continuous drying; Crystallization: nucleation and growth rate, batch crystallizer. **Course Reference:** 1. R. E. Treybal, Mass Transfer Operations, 3rd ed., McGraw Hill, New York, 1980. 2. J. D. Seader and E. J. Henley, Separation Process Principles, Wiley, New York, 1998. 3. J. M. Coulson and J. F. Richardson, Chemical Engineering, Vol. I (6th ed., 2000), Vol. 2 (4th ed.,1990), Vol. 6 (3rd ed., 2000), Butterworth Heinneman, Oxford. 4. B. K. Dutta, Principles of Mass Transfer and Separation Processes, Prentice-Hall of India Pvt Ltd, 2007. 6 5. P.C. Wankat, Separations in Chemical Engineering: Equilibrium Staged Separations, Prentice Hall, NJ. US, 1988 6. McCabe, Smith, and Harriot, Unit Operations in Chemical Engineering, 3 rd ed. McGraw Hil
ChE221	CHEMICAL ENGINEERING THERMODYNAMICS.	3-0-3-0-12	Laws of Thermodynamics: Introduction, Work, Heat, Internal Energy, the first Law, Reversibility, the second law, Entropy, Fundamental Equations: Thermodynamics calculus, thermodynamics derivatives, Euler's theorem for homogeneous functions, Legendre's transformations, Derivative in terms of measurable properties, Equilibria and stability: Equilibrium criteria, stability criteria, Maxwell construction, binodals, spinodals, Gibbs Phase Rule, Clapeyron equation and vapor pressure correlations Pure component properties: Equation of state, Ideal gas heat capacities, fundamental equations from experimental data, fugacity

			and corresponding states Mixture Properties: Mixing function, partial molar quantities, Gibbs-Duhem relation for mixtures, partial Molar quantities from experimental data, Ideal gas mixtures and fugacities, ideal mixtures and activities, excess functions, excess Gibbs free energy models, infinite dilution properties and Henry's Law Phase Equilibria of Mixtures: VLE, LLE, VLLE, Phase equilibria EOS, Osmotic pressure and Osmotic coefficients, Boiling point elevation and freezing point depression Chemical Reaction Equilibria: Reaction extent and Independent reactions, equilibrium criteria and equilibrium constant, reaction standard enthalpies and Gibbs free energy, temperature and pressure effects on reactions, heterogeneous reaction, multiple chemical reactions. **Course Reference:** 1. Engineering and Chemical Thermodynamics, M. D. Koretsky, Wiley India (2004) 2. Essential Thermodynamics: An undergraduate textbook for chemical engineers, Athanassios Z Panagiotopoulos, Drios Press (2011) 3. Chemical Engineering Thermodynamics, by Smith, van Ness and Abbott, 7th Ed., McGraw-Hill (2005) 4. Thermodynamic and Introduction to Thermostatistics, H. B. Callen, 2nd Edition Wiley India (2005). 1. Chemical, Biochemical and Engineering Thermodynamics, S. I. Sandler, Wiley (2006) 2. Chemical Engineering Thermodynamics, Y. V. Rao, Universities Press, India (1997) 3. Chemical Engineering Thermodynamics - Theory and Applications, R. Ravi, Ane Books (2019).
ChE251	INTRODUCTION TO CHE + PROCESS CALCULATION	3-0-3-0-12	Steady-state Material Balances in Non-reacting Systems, Balances on Multiple-Unit Processes, Balances in Reacting Systems, Element (atomic) versus Species (molecular balances), Material Balances in Multiphase Systems, General Energy Balance, Energy Balances in Reacting Systems, Fuels and Combustion, Psychrometry, Unsteady-state material and energy balance. **Course Reference:** 1. "Elementary Principles of Chemical Processes", R. M. Felder and R. W. Rousseau, 2nd ed., Wiley, New York, 1986. 2. "Basic Principles and Calculations in Chemical Engineering", D. M. Himmelblau, 7th ed., Prentice-Hall of India Pvt. Ltd., New Delhi.
ChE261	CHEMICAL PROCESS INDUSTRIES	3-0-0-0-9	Overview of Chemical Industries, Introduction to reactors, Petroleum refining process, Inorganic bulk chemicals, Fertilizers, Hydrogen generation from natural gas, Paper and pulp industry, Modern chemical processes, Petroleum and Petrochemicals. **Course References:** 1. J. H. Gary, G. E. Handwerk and M. J. Kaiser "Petroleum Refining: Technologies and Economics", 5th Edition, CRC Press 2. Kirk-Othmer Encyclopedia of Chemical Technology. 3. Ullmann's Encyclopedia of Industrial Chemistry. 4. Riegle's Handbook of Industrial Chemistry and Biotechnology, Editor: J.A. Kent, 11th edition. 5. Jacob. A. Moulijn, Michiel Makkee, "Chemical Process Technology" 2nd edition.
ChE311	TRANSPORT PHENOMENA: FUNDAMENTALS AND APPLICATIONS	3-0-3-0-12	Fluid flow - Derivation of governing equations using Reynolds Transport Theorem; unidirectional laminar flows, unsteady flows, nearly 1D flows, 2D flows.Heat transport - Governing equations; unsteady conduction in a cylindrical rod; Free and forced convection. Mass transport - diffusion in a stagnant film, diffusion with homogeneous/heterogeneous reactions, diffusion into a falling liquid film. Boundary layer theory and turbulence. **Course Reference:** 1. R. Byron Bird, Warren E. Stewart, Edwin N. Lightfoot, "Transport Phenomena", Second Edition, John Wiley and

			Sons, Inc. 2. V. Kumaran, “Fundamentals of Transport Processes with Applications”, Cambridge-IISc Series, October 2022 (ISBN: 9781009036658). 3. William M. Deen, “Analysis of Transport Phenomena”, Second Edition, Oxford University Press, 2012, ISBN: 9780199740253. 4. L. Gary Leal, “Advanced Transport Phenomena- Fluid Mechanics and Convective Transport Processes”, Cambridge University Press. 5. Rutherford Aris, “Vectors, Tensors and the Basic Equations of Fluid Mechanics”, Prentice Hall International. 5. William B. Krantz, “Scaling Analysis in Modeling Transport and Reaction Processes”, John Wiley and Sons, Inc.
ChE331	CHEMICAL REACTION ENGINEERING	3-0-3-0-12	Introduction; basic concepts in chemical kinetics; determination of rate expressions; nonelementary homogeneous reactions; isothermal design of batch, mixed flow and plug flow reactors; design for multiple reactions; nonisothermal reactors; analysis of nonideal reactors; catalysis; kinetics of catalytic reactions; diffusion and reaction in porous catalysts. **Course Reference:** 1. H. Scott Fogler, ‘Elements of Chemical Reaction Engineering’, 5th edition, 2016, Prentice Hall of India, New Delhi. 2. O. Levenspiel, ‘Chemical Reaction Engineering’, 3rd edition, 1999, Wiley-Eastern Ltd. 3. J.M. Smith, “Chemical Engineering Kinetics,” 3rd edition, 1981, McGraw-Hill, International Student Edition. 4. Unit Operation Laboratory Manual. 5. W.L. McCabe, J.C. Smith, and P. Harriott,” Unit Operations of Chemical Engineering” (7th Edition), McGraw Hill Publishing, 2005 (ISBN 0-07-284823-5). 6. Coulson and Richardson’s Chemical Engineering: Chemical Engineering Design. 7. Bruce A. Finlayson, ‘Introduction to Chemical Engineering Computing’, 2nd edition, 2014, Wiley. 8. Riccardo Tesser, Vincenzo Russo, “Advanced Reactor Modeling with MATLAB: Case Studies with Solved Examples” 2021, De Gruyter.
ChE352	CHEMICAL PROCESS SYNTHESIS AND DESIGN	3-0-3-0-12	Introduction to process design and process creation Heuristics for Process Synthesis Cost accounting and capital cost estimation, annual costs, discounted cash flow analysis, Depreciation Reactor design and reactor network synthesis, Principles of attainable regions, Principles of Reaction Invariants, Optimal reactor conversion and yield, Heat removal configurations, Locating the Separation Section with respect to the Reactor Section, Tradeoffs in processes involving recycle, Recycle to extinction, Influence of side reactions on overall process design, Material and energy recycle and associated non-linear effects: Snowballing, robust flow sheet convergence Conceptual distillation design: sequencing columns for separation of ideal VLE systems. Ternary distillation: feasible splits and design, Complex columns for energy efficiency using state task networks. Non-ideal VLE and residue curve maps, Homogenous azeotropic distillation design, heterogenous azeotropic distillation design, pressure swing distillation, solvent selection Introduction to heat and power integration, Minimum utility targets, networks for maximum energy recovery, minimum number of heat exchangers, threshold and optimal approach temperature, superstructure for minimization of annual costs, multiple utilities and heat-integrated distillation trains. Plantwide Controllability Assessment, Tradeoffs between steady state optimum design and controllability, Design for good operability Lifecycle Analysis.

			Course Reference: 1. W. D. Seider, J. D. Seader and D. R. Lewin, "Product and process design principles", John Wiley (Indian Edition), 2nd edition, 2005 2. M.F. Malone and M. Doherty, "Conceptual Design of Distillation Systems", McGraw-Hill, 1st Edition, 2000. 3. Robin Smith, Chemical Process Design and Integration, 2nd edition, John Wiley and Sons, Inc.
ChE362	BIOCHEMICAL ENGINEERING	3-0-01-4	Cell Structure and Cell Types, Chemicals of Life (RNA, DNA, enzymes etc.), Kinetics of Enzyme Reactions, Applied Enzyme Catalysis, Metabolic Stoichio metric and Energetics, Molecular Genetics and Control, Biomass Production, Transport Phenomena in Biosystems, Design and Analysis of Biological Reactors, Fermentors, Downstream Product Recovery and Purification, Interaction of Mixed Microbial Populations, Biological Wastewater Treatment.
ChE381	PROCESS DYNAMICS AND CONTROL	3-0-3-0-12	Basic SISO dynamic elements; Solving ODEs in time-domain; Characteristic equation and stability; Empirical dynamic modelling of SISO systems; First-principles dynamic modelling and simulation; SISO negative feedback control; PID control algorithm, stability and tuning; Laplace-domain techniques: Laplace transform, transfer functions, partial fractions, root locus technique, direct synthesis and internal model controller design; Frequency-domain techniques: The frequency response, Bode and Nyquist plots, Nyquist stability theorem, controller tuning for gain margin, phase margin and maximum closed loop sensitivity; Multivariable systems: Interaction metrics (relative gain array and Niederlinski Index), decentralized PID controller (de)tuning, decoupling; Advanced control: Feedforward, Ratio, Cascade, Optimizing, Override; Model based control: Smith-predictor, model predictive control; Control system design for complete plants; Digital control analysis and design. **Course Reference:** 1. Process Control: Designing Processes and Control Systems for Dynamic Performance, 2nd Ed, TE Marlin (2000). 2. Essentials of Process Control, WL Lubyen and ML Luyben (1997). McGraw Hill: New York. 3. Process Dynamics and Control,4th Ed., DE Seborg, TF Edgar, DA Mellichamp and FJ Doyle III, (2016). John Wiley and Sons: Hoboken NJ.
ChE391A	UNIT OPERATION LABORATORY -I	1-0-3-2-8	Safety, ethical guideline, error analysis, data presentation. Brief introduction to topics of experiments, relevance in industry Fluid flow, fluid particle system Thermodynamics Heat and mass transfer Demonstration lab Solid size reduction e.g. crushing and Igrinding, ball milling; Solid conveying e.g. pneumatic conveying, hydraulic conveying, Ibelt conveying. Analysis and testing of crude oil and petroleum products: 1Determination of octane number, cetane number, pour point, cloud point, smoke point **Course Reference**: 1. Unit Operation Laboratory Manual; 2. Unit Operations of Chemical Engineering; (7th Edition), by W.L. McCabe, J.C. Smith, and P. Harriott, McGraw Hill Publishing, 2005 (ISBN 0072848235); 3. Coulson and Richardson's Chemical Engineering: Chemical Engineering Design
ChE453	PROCESS DESIGN CAPSTONE PROJECT	0-1-4-0-6	Validation of thermodynamic properties, Validation of kinetic parameters, Steady State flow sheet synthesis, Economic optimization, Heat Integration, Plant wide control. **Course Reference:** 1. J. M. Douglas, "Conceptual design of chemical processes", McGraw-Hill, 1988. 2. W. D. Seider, J. D. Seader and D. R. Lewin, "Product and process design principles",John Wiley (Indian Edition), 2nd edition, 2005. 3. M.F.

			Malone and M. Doherty, “Conceptual Design of Distillation Systems”, McGraw-Hill, 1st Edition, 2000. 4. Robin Smith, Chemical Process Design and Integration, 2nd edition, John Wiley and Sons, Inc. 5. G. Towler and R. Sinnott, Chemical Engineering Principles, Elsevier, 2008.
ChE454A	UNIT OPERATIONS INVOLVING PARTICULATE SOLIDS FOR CHEMICAL ENGINEERS	3-0-0-0-9	Particles Size Analysis: Sieve analysis, size distribution, size averaging and equivalence, size estimation in sub-sieve range, effectiveness of screen, description of shape and morphology of particles (flocs, porous particles, surface texture etc.), Size Reduction: Theory of crushing and grinding, laws of crushing and grinding, crushing and grinding equipment and their selection,Nanoparticles: Synthesis, characterization and potential applications, enlargement of particles by agglomeration and other methods,Storage of Solids: Angle of slide and repose, general design consideration for bins, silos and hoppers,Particle Mechanics: Motion of particle in fluid, pressure-drop calculations for solidliquid slurry flow, effect of particle shape, Stoke’s law, hindered settling and jigging,Sedimentation and Flotation: Gravity and centrifugal sedimentation, design of sedimentation tank and continuous thickeners, mechanism of flotation, flotation agents and flotation equipment,Fluidization: Fluidization characteristics, aggregative and particulate fluidization, voidage and minimum fluidization velocity, voidage correlation, liquid-solid and gassolid fluidization characteristics, industrial applications of fluidization,Filtration: Flow through filter cake and medium, washing and drying of cake, filter aids, selection of filtration equipment, constant rate and constant pressure filtration, Other Separation Equipment: Cyclone separator, air filter, electrostatic separator, and their design consideration,Conveying of Solids: Pneumatic and hydraulic conveying of solids, general characteristics and flow relations, mechanical conveyers
ChE611	TRANSPORT PHENOMENA	3-0-0-0-9	Kinematics, Transport theorem, constitutive relations, Equations of motion and their solutions, Boundary layer theory, Turbulence; Energy equation and its exact solutions, Continuity equation for multicomponent systems, constitutive relations, Interphase transport of momentum, energy and mass and macroscopic balances.
ChE614	INTRODUCTION TO HYDRODYNAMIC STABILITY	3-0-0-0-9	Introduction; Notions of stability (Lyapunov stability; asymptotic stability; spatial vs temporal instability; transient growth etc.); Review of governing equations of fluid flow and boundary condition; Instabilities in fluids at rest (Rayleigh-Taylor instability, Rayleigh-Plateau instability) Rayleigh-Benard instability, Marangoni thermocapillary instability); Kelvin- Helmholtz instability; Stability of parallel shear flows; Inviscid limit (Rayleigh, Fjortoft theorems); Viscous flows: Squire’s theorem; Orr- Sommerfeld equation for rectangular and axisymmetric geometries; Numercal techniques for solving the Orr-Sommerfeld equation; Interfacial instabilities in multi-layer flows; Spatio-temporal evolution(convective vs absolute instabilities); Non-modal analysis and transient growth; Weakly non-linear stability; Instabilities n non-Newtonina fluids.
ChE616A	INTRODUCTION TO GRANULAR MECHANICS	3-0-0-0-9	Part:1 Introduction to granular materials (Illustrative examples, rich behaviour of granular materials, characterisation of granular materils, inter-particle forces, fluid paricle interaction); Issues and challenges in experimental studies; Discrete element method for granular simulations; Hard and soft particle models; Contact force

			modelling (Normal contact force models, tangential contact force and torque models, Friction force modelling, Equations of motion for granins (non-dimensionalizaion of equaitons of motion, relating model parameters to grain properties); Algorithm for soft and hard particle mehods; Calculation of varios properties of interest form the data; Modelling of non-spherical granis in DEM; Some fundamental insights obtained form DEM; Limitation of Dem simulations. Part-2: Cintinuum models (Balance laws for msss, momentum and energy); Static properties of a granular piles (Role of friction, Reynolds dilatancy, Pressure distribution in cylindrical container); Theory of slow flows (Coulomb yield condition, Mohr's Circle, Rankine states, Flow rules, Equations for plane flows); Flow thorugh hoppers and wedge shaped bukers (Savage's smooth wall radial gravity solution, Beverloo correlation of flow through cylindrical silos with circular orifice and it's theoretical estimation); Rapid flow of smooth, inelastic granins in simple geometries (Hydrodynamic description of rapid granular flow, Heuristic theory and introduction to Kinetic theory of inelastic gases). Par 3: Dense granular flow rehlogy (Frictional kinetic hybrid model, Local rehlogy vs. non-local rehelogy, inertial-number rheology in dense flow regime, 3D viscoplastic rheological model, extension to the rheology of granular mixures); Surface flows of granular materials (Flow over inclined plane and in rotating cylinders and heaps, depth average equation for surface flows); Mixing and segregation of granular mixtures (Savage's kinetic sieving mode, Khakhar's single particle based segregation mode, kinetic theor based segregation models).
ChE619A	ADVANCED FLUID MECHANICS	3-0-0-0-9	Introduction,Review of basic mathematical tools (vector calculus,theorem's of integral calculus),Kinematics-Continuum hypothesis, Reference frames (Lagrangian vs Eulerian), General balance equations-Continuity,Conservationof linearmomentum,Interfacial transport, Angular momentum equation, Stream function and velocitypotential,Analysis ofUnidirectional and nearly unidirectional flows; Lubricationapproximation: application to thin films, Creeping flow with focus onMicrohydrodynamics:solution techniques using expansions of harmonic and Green's functions;Resistance matrices;singularitysolutions;flows involving rigid particles and fluid droplets; applications tosuspensions,Laminarflow athigh Reynold's number–Inviscid flow, irrotational flow, Idealflows in a plane,Axisymmetric ideal flows,Vortex dynamics:Concept of vorticity;Kelvin's Circulation Theorem;Helmhotz'sVortex Theorems;Vorticity Equation in a Nonrotating Frame;Vortex Sheet,Boundary Layers: Blasius Flow ever a Flat Plate,Displacement Thickness,VonKármán Momentum Integral,Von Kármán-Pohlhausen Approximate Method,Falkner-Skan Similarity Solutions,Arbitrary Two-Dimensional Lay: Crank-Nicolson Difference Method,Introduction to Turbulent Flows: Types of Turbulent flowsandtheircharacteristics, Reynolds Stress, Correlations of fluctuations, Meanand TurbulentKinetic energy, Energy Cascade (Kolmogorove scalesand Taylor microscale)
ChE623A	THERMODYNAMICS OF FLUIDS AND FLUID MIXTURES	3-0-0-0-9	Classical thermodynamics of phase equilibria: Thermodynamic properties from volumetric data: Nature of intermolecular forces, Theory of corresponding states; Fugacities in gas mixtures and liquid solutions; gas solubilities; High pressure equilibria.

ChE626	PRACTICAL INTRO. TO QUANTUM MECHANICAL METHODS FOR SCIENTISTS & ENGINEERS	3-0-0-0-9	Summary of classical mechanics: conservation laws, Hamiltonian and Lagrangian formulation; The need for quantum mechanics; Basic concepts: physical observables and operators, expectation values, Heisenbergr's uncertainty principle, Schrodinger's equation; The many-body Hamiltonian, Born-Oppenheimer ¨ approximation, variational principle, the concept of potential energy surface; What makes electronic structure difficult; Hartree-Fock (HF) approach: restricted and unrestricted method, and their comparison with experiments; Localized and plane-wave basis sets; Pseudopotentials; Density functional theory (DFT): Hohenberg-Kohn theorems, Kohn-Sham formulation; Exchange and correlations: LDA and GGA approximations; Pure and hybrid DFT functionals; Tricks for self-consistent solution of the Kohn-Sham system: mixing and diagonalization techniques; Failures and successes of DFT: vander Waal's correction and DFT+U approach; Configuration interaction and Miller-Plesset perturbation theory; Applications of quantum-mechanical methods in engineering and sciences; Specialized topics (if time permits): Ab initio molecular dynamics (Born-Oppenheimer and Car-Parrinello), ring-polymer molecular dynamics.
ChE631A	CHEMICAL REACTION ENGINEERING	3-0-0-0-9	Behaviour of chemical reactions; Behaviour of chemical reactors: ideal and nonideal flow, nonisothermal reactor performance, reactor stability; Heterogeneous reactions: interphase and intraphase heat and mass transfer effects; Fluid Solid noncatalytic reactions; Heterogeneous catalytic reactions.
ChE635A	INTRODUCTION ELECTROCHEMICAL ENGINEERING	3-0-0-0-9	Overview of electrochemical engineering; Thermodynamics of electrochemical systems; Electrochemical kinetics, electrocatalysis and models for electron transfer; Transport in electrochemical systems; Engineered & selforganized electrode macro, microand nanoarchitecture; Electrochemical measurements and overview of electroanalytical chemistry; Fundamentals of electrochemical biosensors & electrophysiology; Fundamentals of batteries; Fundamentals of fuel cells; Fundamentals of electrochemical capacitors; Fundamentals of photoelectrochemical systems and semiconductor electrochemistry; Fundamentals of electrodeposition and current distribution in electroplating; Fundamentals of electroless deposition and corrosion; Electrochemical reactor & process engineering
ChE636A	NUMERICAL SIMULATION OF FLUID FLOW THROUGH POROUS MEDIA	3-0-0-0-9	Introduction to porous media; Fluid and rock properties, Fundamental fluid flow equaions in porous media, Overview of finite difference methods for partial differential equaitons, Single phase flow throuth porous media, Numerical simulation of single phase flow, Two phase immiscible displacement; Buckely-Leveret theory for immiscible displacement; Numerical simulation of tow-phase immiscible displacement, Special topics (CO2 sequestration, groundwater flow, oil recovery, fuel cells, biological applications, etc.)
ChE638A	MICROWAVE AND PLASMA CATALYSIS, REACTION AND REACTOR ENGINEERING	3-0-0-0-9	Energy scales of molecule & methods of activation: Thermochemical, electrochemical, photochemical Vs. Electrodynamical; Review of Maxwell's equations; Basis for energy scales within the molecule: Review of elementary quantum

			mechanics; Temperature and Energy distribution: Review of elementary statistical mechanics; Microwave & Chemical phenomena; Interaction of Microwave with Dielectric materials; Hot spots and excitations; Coupling microwave with heterogeneous catalysts; Transport phenomena in microwave systems; Microwave reaction kinetics and reactor design; Heuristics for microwave catalytic process design; Electrodynamics of Charged Species in Plasma; Electron transfer in heterogeneous systems at high electrochemical potentials; Excitation of Molecules and Atoms in Plasma; Statistics and Kinetics of Charged Particles in Plasma; Kinetics of Excited Particles in Plasma; Transport in plasma system; Microwave plasma catalysis; Physicochemical phenomena with Glow & Arc discharge; Heuristics for Plasma catalytic process design
ChE642A	NUMERICAL METHODS IN CHEMICAL ENGINEERING	3-0-0-0-9	Systems of Linear and NonLinear Algebraic Equations: Successive Substitution, Newton Raphson, Eigenvalues and Eigen vectors of Matrices, Interpolation, Solutions of ODEs (IVP): Runge Kutta, Multistep Methods, Gears algorithm, Stiffness and Stability of algorithms, ODE (BVPs) and PDEs: Finite Difference, Finite Elements, Shooting Methods.
ChE643A	MESOSCALE AND CONTINUUM SIMULATIONS IN CHEMICAL ENGINEERING	1-0-6-0-9	Introduction to particle-based simulation, Newtons laws of motion, Molecular Dynamics, Langevin dynamics, Brownian dynamics, 1D random walk with MSD calculation, Stokes-Einstein, length and timescales accessible; Polymer chain statistics, radius of gyration, Rouse and Zimm models, normal mode analysis; Finite difference method, Numerical Integration; Algorithms in MD/BD: Verlet and related integration schemes, Linked Lists, Neighbor lists
ChE652	OPTIMIZATION	3-0-0-0-9	Mathematical formulation of optimization problems; single variable problems: search techniques; Multivariable problems without constraints: direct methods, first and second order methods; Multivariable problems with constraints: Calculusof variations; Pontryagins maximum principle; Dynamic Programming.
ChE655A	DATA SCIENCE FOR CHEMICAL ENGINEERS	3-1-3-0-12	Introduction to Data Science, Data Source and Examples of Data Type, Vector Spaces: Four fundamental spaces: eigenspace, Singular Value Decomposition (SVD), Optimization: Steepest descent, conjugate gradient, con-strained optimization, Machine Learning Techniques: Least squares and non-linear least squares, Principal Component Analysis (PCA), Support-Vector Machines (SVM), Partial Least Squares (PLS), Time Series Analysis :Linear stationary and nonstationary models, forecasting, identi_cation, estimation and diag-nostics, minimum variance control, Neural Networks: Multilayer perceptron, Backpropagation NN, Radial Basis, unsupervised learning networks, applications
ChE656A	MATERIALS TO PRODUCT: DESIGN & ENGINEERING	3-0-0-0-9	Introduction to Chemical Product Design & Engineering - What, Why & How?; Case studies: materials and devices during the covid crisis (medical oxygen generators), Freon, Nylon, Penicillin, Taxol, tasty chocolates, water purifiers, explosion-free batteries, Fuel-cell catalysts, Biofuels; Selection of materials/products: selection using thermodynamics, selection using kinetics, risk assessment & management; Material properties: mechanical, electrical, optical, thermal, etc.; From chemical to material phase diagrams; Estimating properties of materials: Theory (Quantum Chemical Descriptors, Statistical Thermodynamical Methods), Correlations (classification,

			regression, empirical), Structure-Property relationship; Measuring properties of materials: structural, morphological, optical properties, etc.; General Principles of Material processing; Correlating properties to structure and processing; Product Design: safety & environmental concerns, green processes; Product Engineering: materials failure, scaleup etc.; Product marketing and economics: customer needs, market size, business plan
ChE664	ELECTROCHEMICAL ENERGY CONVERSION AND STORAGE	3-0-0-0-9	I.Introduction to electrochemical energy conversion and storage devices (2weeks); a. Contemporary energy challenges and opportunities; b. Advantages and disadvantages in electrochemical approach to energy conversion and storagec. Qualitative introduction to fuel cells; Photoelectrochemical cells, batteries, supercapacitors and thermoelectric devices; 2. Thermodynamics of electrochemical systems (2 weeks) a. Electrochemical potential b. Activity coefficientsc. Reference electrodesd. Junction potential; 3. Electrodics (3 weeks) a. Electrochemical double layer b. Electrode kineticsb. Electrode kinetics; 4. Transport processes in electrochemical systems (3 weeks) a. Transport in diiure soiutionsb. Transport in concentrated solutions. Transport phenomena in electrochemically reactive systems5. Electrochemical measurements (I week) a. Cyclic voltametry b. Impedance spectroscopy. Scanning probe techniques 6. Design issues in electrochemical energy devices (3 weeks) a. Current distribution in Fuel cells and Batteriesb. Material design strategies for electrodes/electrolytes c. Economics of Electrochemical devices. **Course Reference**: 1. Newman, J. and Thomas Aiyea, K., Electrochemical systems, WileyInterscience (2004); 2. Larminie, J. and Dicks, A., Fuel cells systems explained, JohnWiley & Sons (2003); 3. Linden, D. ed., Handbook of Batteries, McGrawHill (2001); 4. Bard, A. and Faulkner, L.R, Electrochemical methods, JohnWiley & Sons(2001); 5. Bockris, J.O.M. and Reddy, A.K.N., Modern Electrochemistry (Volume 1, Volume 2A and 2B),Springer (2001); 6. Course materials will be supplemented with research and reviews for journals.
CHE667A	PRINCIPLES OF NON-NEWTONIAN FLUID MECHANICS	3-0-0-0-9	Course Contents: 1. Introduction a. Effects and phenomena in non-Newtonian fluid mechanics b. Vector and tensor operations c. Overview of Newtonian fluid mechanics 2. Standard flows for non-Newtonian fluids a. Simple shear flow b. Simple elongational flows – uniaxial, biaxial and planar elongational flows c. Forms of stress tensor in standard flows 3. Material functions for non-Newtonian fluids a. In steady and unsteady shear b. In steady and unsteady elongational flow 4. Overview of experimental data a. Flow response in steady and unsteady shear flow i. Effects due to structure of material ii. Effects due to temperature and pressure iii. Small and large strains b. Flow response in steady and unsteady elongational flows i. Small and large strains

			5. Constitutive models without memory effects – Generalized Newtonian Fluids (GNF) a. GNF constitutive models i. Power-Law model ii. Carreau-Yasuda model iii. Bingham model b. Predictions of material functions c. Flow problems d. Limitations 6. Constitutive models with memory effects – Generalized Linear Viscoelastic (GLVE) fluids a. Memory effects b. Maxwell models c. Generalized linear viscoelastic model (GLVE) d. Flow problems with GLVE constitutive model e. Limitations 7. Advanced constitutive modeling a. Finite strain measures – deformation, finger and Cauchy tensors b. Lodge equation c. Convected derivatives d. Other constitutive models i. Continuum approaches ii. Molecular approaches 8. Introduction to numerical methods in non-Newtonian fluid mechanics a. Discretization schemes – finite difference, spectral and finite elements b. Solution procedures and stabilization c. Few test problems
CHE668A	BIOPROCESS ENGINEERING	3-0-0-0-9	Introduction, Basics of Biology (Biochemistry, Genetics, etc.); Metabolism, Metablic Pathways, Metabolic Regulation, Stioichiometry, Enzyes: Nomenclature, Classification,Examples, Enzyme Kinetics, Enzyme Inhibition, Allosteric Interaction, Enzyme Immobilization and Mass Transfer Effects, Cell Growth: Phases, Batch Kinetics, Quantifying Batch Growth Kinetics, Unstructured and Structured Modesl of Growth; Cell Growth: Continues, Chemostat, Chemostat with Recycle; Reactor Operations: Sterilization, Batch and contiunuous operation, Aeration, Heat and Mass Transfer in Reactors; Bioreactor Monitoring and Control: DO, pH, T, Off Gas, Substrate etc. Recovery and Purification: Extracellurlar Product Recovery, Filtration, Centrifugation, Coagulation, Flocculation; Recovery and Purification: Cell Disruption Techniques, Intracellurlar Product Recovery, Extraction, Adsorption, Ultrafiltration, Chromatography, Crystallization etc; Mixed Cultures; Classes of Interaction, Simple/Classical Models; Mixed Cultures: Industrial Utilization – Defined and Undefined Mixed Microbial cultures

ChE673	ENVIROMENTAL POLLUTION CONTROL, DESIGN AND MODELLING	3-0-0-0-9	1. Air Pollution: a. Introduction: Atmospheric pollutants: definition, sources, concentration levels, units. b. Gaseous phase chemistry: photochemical smog in troposphere; O3 depletion in stratosphere; NOx formation in urban atmosphere, PAN/PAH formation. c. Aqueous phase chemistry: acid rain (SO2, CO2, NO2), Chemical equilibria.d. Aerosols: size, distribution, deposition, visibility degradation, nucleation. f. Mass transfer aspects: diffusion, mass transfer coefficient, characteristics times. g. Troposphere energy balance: pressuretemperature relationship, stability criteria, rising parcel of air pollutants, stack plume rise. h. Atmospheric dispersion: puff and plume dispersion, Gaussian models. i. Control of Pollutants: (1) Absorption: design of an absorber (SO2, CO2, NO2) (2) Adsorption: design of an adsorber (SO2, VOC), breakthrough analysis (3) Particles: mechanism of particles capture, fabric filters, cyclones, precipitator2. Water Pollutiona. Introduction: organic/inorganic/biological pollutants, water quality and parameters. b. Waste water treatment: primary and secondary treatments, sludge disposal (aerobic and anaerobic digesters. c. Biological organic wastes: BOD/COD, dissolved O2 model, Monods kinetics, biomass growth & food utilization. d. Biological wastewater treatment equipment design: (1) Activated sludge process reactor (2) Trickling filter (3) Biotower reactor. e. Advanced waste water reactors: (1) Continuous counter current multi stage fluidized bed. (2) Moving bed adsorption systems. **References/Text Books:** 1. Atmospheric Chemistry and Physics by Seinfeld and Pandis (Wiley.) 2. Environmental Engineering by Peavy, Rowe, and Tchobanoglous (McGraw Hill.)
ChE677A	INTRODUCTION TO PHYSICS OF POLYMERIC SYSTEM	3-0-0-0-9	Introduction to Polymers a. What are polymers ? b. Molecular Weights and their averages 2. Polymer conformations of ideal chains a. Conformations b. Bond rotation and Polymer size c. Persistence length and Kuhn Length d. Distribution of end to end distance e. Radius of gyration f. Self-avoiding chains and excluded volume effect. 3. Thermodynamics of Poylmer Solutions a. Review of concepts of Thermodynamics and Statistical Mechanics b. Regular solution Theory c. Flory Huggins theory d. Phase behaviour of polymer solutions and blends e. Concentration regimes 4. Light scattering a. Basic concepts of scattering b. Scattering by an isolated molecule c. Scattering by dilute polymer solution d. Form factor and Zimm equation e. Other techniques 5. Rhelogy of polymer solutions and molecular theories a. Introduction to viscosity, modulus and normal stress differences b. Intrinsic viscosity c. Linerar vs Non-linear response d. Maxwell model and Boltzmann superposition principle e. Bead-spring model f. Zimm model for dilute solutions g. Rouse theory for unentagled melts h. Reptation model for entangled melts 6. Glass Transition a. Introduction to transitions in pure polymers b. Amorphous vs glassy polymers c. Thermodynamics aspects of the glass transition d. Free volume description e. Time temperature superposition f. Glass transition in

			thin films 7. Composite systems a. Introduction to composite systems b. Dispersion of colloids in polymer solutions c. Diffusion of colloids in polymer solutions d. Influence on Glass transion e. Static Light Scattering of composites.
ChE678A	MECHANICS OF SOFT MATERIALS	3-0-0-0-9	1. Fundamental Equations: The strain tensor; The stress tensor; Thermodynamics of deformation; Hooke's law; Homogeneous deformations; Equilibrium of an elastic medium bounded by a plane; Solid bodies in contact with and without interactions. (10 hours); 2. Equilibrium of rods and plates: Equations of equilibrium of rods; Bending and torsion of rods. Equation of equilibrium for a bent plate; The energy of a bent plate; Application of bending plate geometry for solving problems related to Adhesion. (10 hours); 3. Nonlinear elasticity: Molecular approach to rubber; strain energy theory; specific forms of strain energy; NeoHookean elasticity. Solutions for incompressible materials. Cavitation in crosslinked networks. (10 hours); 4. Mechanics of cell wall: Elasticity of cellular filaments; soft networks in cell; biomembranes, membrane undulations. (10 hours) **Course Reference**: 1. Theory of Elasticity, 3rd edition by Landau and Lifshitz. Course of theoretical physics, vol7; 2. A treatise on the mathematical theory of elasticity by A. E. H. Love; 3. Contact Mechanics by K. L. Johnson; 4. Mechanics of the cell by David Boal.
ChE679	SPECIAL TOPICS	3-0-0-0-9	Course contents vary from time to time
ChE684A	AN INTRODUCTION TO SYSTEMS BIOLOGY	3-0-0-0-9	Introduction to transcription Networks; The Concept of Network Motif; Autoregulation loops: Positive and Negative autoregulation; Feed Forward loops; Global structure of Transcription Networks and Temporal responses; Network motifs in Development, Signal Transduction, and Neuronal Networks; Robustness of Protein Circuits; Kinetic Proof reading; Optimal gene circuit design; Demand rule for gene regulation; Input function of a Gene: Michaelis Menten and Hill equations, Multidimensional input functions .Duration: One Semester **Course Reference**:1. An Introduction to Systems Biology by Uri A ton. (Chapman & 1Iaii/CRC, UK, 2007); 2. Mathematical Models in Biology by Edelstein Keshet, L. (Cambridge University Press,2005); 3. Systems Biology Properties of restructured Networks by Bernhard 0. Palsson (Cambridge University Press, 2006); 4. Virus dynamics: Mathematical principles of immunology and virology by Martin A. Nowak And Robert may (Oxford University press, USA,2001)
ChE688	FUNDM. OF COLLOID & INTERFACE SCI. & TECH.	3-0-0-0-9	Capillarity, interfacial thermodynamics, surflactants, stability of multiphasesystems, foam, emulsion, multiphase reactors, wetting and adhesion, catalystsintering/redispersion; Stability and coagulation of colloids, nucleation andgrowth: Colloids in chemical engineering, in separation processes, bioscience.
ChE888	INTRODUCTION TO PROFESSION AND COMMUNICATION SKILLS FOR CHEMICAL ENGINEERS	1-0-3-0-6	Introduction to scientific Research: Objectives and nature of scientific research, Scientific thinking, Framing of hypothesis and Karl Popper's falsification principle.; Ethics in research and publishing: Academic Integrity, data sharing, transparency, authorship, giving credit, disclosure, Misconduct in research vis-a-vis honest errors; Writing scientific documents: Reports, papers, and thesis formats. Popular and Formal scientific communication. English for Scientific writing, Literature search and review; Tools for academic writing and publishing: Writing tools (Latex, MS word etc.),

			Proofreading tools, Reference manager, Plotting and data analysis tools, etc.; Effective oral communication and tools: Presentation skills, Effective usage of slidesetc.; Exposure to intellectual property: Patents, copyright etc.; Professional opportunities after PhD: Academia, R&D in Industry and National Labs, Non-academic professional options, Start-up etc.
ChE801	GRADUATE SEMINAR	----0	Graduate Seminar
ChE801A	GRADUATE SEMINAR		To be Procured
ChE802	GRADUATE SEMINAR	----0	Graduate Seminar
ChE802A	GRADUATE SEMINAR		To be Procured
ChE666	Stability Theory for Chemical Engineers	3-0-0-0 [9]	The objective of this course is to familiarize students with the applications of non-linear dynamics and stability theory in various aspects of core chemical engineering. Recommended pre-requisites, if any: CHE212, CHE213, CHE331 **Short summary for including in the Courses of Study Booklet:** Introduction to stability theory, lumped parameter systems with ODEs, saddle-node, transcritical, pitchfork bifurcations, 2D Systems - fixed points, phase plane, eigenval- ues, eigenvectors, conservative systems, Lotka-Volterra, limit cycles, non-isothermal CSTR, multi-component distillation, residue curve maps, distillation boundary, oscillating reactions, distributed parameter systems with PDEs, modal analysis, dispersion relations, Turing patterns, stability of PFR, spatiotemporal chemical oscillations **Recommended text/reference books:** *Strogatz SH. Nonlinear dynamics and chaos: with applications to physics, biology, chemistry, and engineering. CRC press; 2018.* *Perlmutter DD, Stability of Chemical Reactors. Prentice-Hall; 1972.* *Doherty MF, and Malone MF. Conceptual Design of Distillation Systems. McGraw-Hill, 2001.* *Cross M, Greenside H. Pattern formation and dynamics in nonequilibrium systems. Cambridge University Press; 2009.* *Epstein IR, Pojman JA. An introduction to nonlinear chemical dynamics: oscillations, waves, patterns, and chaos. Oxford university press; 1998.*
ChE682	Applied Machine learning for Chemical Engineers	3-0-0-0 [9]	Course Description: Objectives: The course will attempt to introduce the essential concepts and tools of Machine learning with an emphasis on applications. Frequent computer assignments will further enforce practical learning of the same and show possible usage in engineering, particularly chemical engineering, applications.

Contents (preferably in the form of 5 to 10 broad titles): Lecture-wise break-up (considering the duration of each lecture is 50 minutes)

Sl No	Broad Title	Topics	No. of Lectures
1.	Introduction	Introduction to Machine learning and basics of python programming	3
2.	Optimization tools	Zero order, first and second order optimization techniques	7
3.	Linear learning	Linear regression, least squares and least absolute deviations, multi-output regression	5
4.	Linear learning Linear two-class	Logistic regression: Cross Entropy and Softmax cost, Perceptron, Support Vector Machines	8
5.	Multi-Class classification	One-versus-all multi-class classification, Multi-class Perceptron	4
6.	Linear Unsupervised learning	Spanning sets, orthonormality, projections, Principal component Analysis, Recommender systems, K-means clustering, Matrix Factorization problems	6
7.	Non-linear learning	Non-linear regression, non-linear two-class classification, non-linear multi-class classification, non-linear unsupervised learning	4
8.	Fully connected Neural Networks	Basics of Neural Networks	3

Recommended pre-requisites, if any (examples: a- PS0201A,or b-PS0201A or
equivalent): Basic UG-level programming and numerical methods knowledge

Short summary for including in the Courses of Study Booklet:
Optimization Tools, Linear learning methods, Linear classification methods, Linear unsupervised learning, Non-linear learning, Neural networks

Recommended text/reference books:
A) Jeremy Watt, Reza Bohrani, Aggelos K. Kastaggelos, Machine Learning Refined 2nd Ed., Cambridge University Press, 2020.

Any other remarks:

<table>
<tr><td></td><td></td><td></td><td>A) Most of the homework assignments will involve computer programming by the students. Assignments will be given every week.</td></tr>
<tr><td>ChE683</td><td>Foundation of Deep learning for Chemical Engineers</td><td>3-0-0-0 [9]</td><td>Course Description:
Objectives: The course will build up from a basic Machine learning course and introduce the concepts of Deep learning. The students are expected to have a basic exposure of Machine learning and computer programming. The problems and examples relevant to engineering, especially chemical engineering, will be selected, whenever possible.

Contents (preferably in the form of 5 to 10 broad titles): Lecture-wise break-up (considering the duration of each lecture is 50 minutes)

<table>
<tr><th>Sl No</th><th>Broad Title</th><th>Topics</th><th>No. of Lectures</th></tr>
<tr><td>1.</td><td>Introduction</td><td>Introduction to Deep learning and examples</td><td>2</td></tr>
<tr><td>2.</td><td>Probabilities and distributions</td><td>Probability, Probability density, Information theory, Bayesian probabilities, Discrete variables, Multivariate Gaussian</td><td>6</td></tr>
<tr><td>3.</td><td>Single Layer Networks: Regression</td><td>Linear regression, Basis functions, Likelihood function, Geometry of least squares, Multiple outputs</td><td>4</td></tr>
<tr><td>4.</td><td>Single Layer Networks: Classification</td><td>Discriminant functions, Decision Theory, Generative Classifiers, Discriminative Classifiers</td><td>6</td></tr>
<tr><td>5.</td><td>Deep Neural Networks</td><td>Limitations of fixed basis functions, multilayer networks, deep networks, error functions</td><td>6</td></tr>
<tr><td>6.</td><td>Gradient Descent</td><td>Gradient Descent optimization, convergence, normalization</td><td>3</td></tr>
<tr><td>7.</td><td>Backpropagation</td><td>Evaluation of gradients, automatic differentiation</td><td>2</td></tr>
<tr><td>8.</td><td>Convolutional Networks</td><td>Computer vision and convolutional filters, visualizing trained CNNs and object detection</td><td>3</td></tr>
<tr><td>9.</td><td>Graph Neural Networks</td><td>Machine learning on graphs, Neural message-passing, General graph networks</td><td>4</td></tr>
<tr><td>10.</td><td>Sampling</td><td>Sampling algorithms, Markov Chains Monte Carlo, Langevin Sampling</td><td>4</td></tr>
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			Recommended pre-requisites, if any (examples: a- PS0201A,or b-PS0201A or equivalent): Basic UG-level programming and any first level course on Machine learning. Short summary for including in the Courses of Study Booklet: Probability, Distributions, Single layer networks for regression and classification, Deep neural networks, Gradient descent, Convolutional networks, Graph neural networks, Sampling Recommended text/reference books: Christopher M. Bishop, Hugh Bishop; Deep Learning, Springer, 2024. Any other remarks: Most of the homework assignments will involve computer programming by the students. Assignments will be given every week.
CHE669	Chemical Kinetics: Reaction Rate Theories and Rare-Event Simulations	3-0-0-9	Objectives: The goal of the course is to acquaint students with the fundamentals of chemical kinet- ics, rare-event simulations, and reaction rate theories. The course will thoroughly cover the underlying theory and the assumptions made in it, even though the focus will be on applications. This is because understanding this material is essential to being an intelligent practitioner
CHE634	Fluid Dynamics of Microscopic Self-propulsion	3-0-0-0 (9)	**Description:** The ability to predict, control, and design the behaviour of microscopic swimmers such as motile bacteria, synthetic Janus colloids, and medical micro-robots, defines a growing frontier at the intersection of fluid mechanics, biophysics, and engineering. The principles governing locomotion at the micron scale are counterintuitive: fluid inertia is irrelevant, time-reversal symmetry severely constrains what strokes are possible, and a swimmer's fate in confinement is often dictated by the geometry of its far-field signal. This course provides students with the theoretical framework to understand these principles, starting from the fundamental properties of viscous flow to quantitative models of biological and artificial microswimmers. By the end of the course, students will be equipped to independently analyse swimmer kinematics and hydrodynamic signatures, apply the reciprocal theorem and image methods to new geometries, and critically read the current research literature on fluid mechanics of active matter and bio-inspired locomotion.
CHE658	Mathematics for Machine Learning	3-0-0-0-(9)	**Objectives:** The aim of this course is to introduce students to mathematical methods required for Machine learning applications. This is primarily intended for PG students and can serve as a preparation course towards a Machine learning/Deep learning elective. Most topics would be supplemented by computer-based exercises as well. This can also serve as an introductory Machine learning course.
CHE615	Microhydrodynamics and Suspensions	3-0-0-0-(9)	**Objectives:** This course aims to introduce microhydrodynamics leading to macroscopic phenomena in suspension dynamics. The concepts are expected to be useful for dynamics in a variety of systems relevant to chemical engineers, including suspensions, polymer solutions and even biological systems like blood, which is a essentially a suspension of RBCs. The course is aimed primarily

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<tr><td></td><td></td><td></td><td>towards PG students and would consist of computerbased exercises and term projects as well.</td></tr>
<tr><td>CHE602M</td><td>Introduction to Transport Phenomena</td><td>3-0-0-0-(5)</td><td>Objectives: The course will expose fresh PhD students to basic concepts of Transport Phenomena along with some simple examples.
<table>
<tr><th>S. No.</th><th>Broad Title</th><th>Topics</th><th>No.of Lectures</th></tr>
<tr><td>1.</td><td>Vectors, Tensors, and their calculus</td><td>Stress tensor and velocity gradient tensor: Sec 7.3.2 and 7.3.3 of V. Kumaran Gradient, Divergence and Curl: Appendix 7A, 7B, and 7C of V. Kumaran</td><td>2</td></tr>
<tr><td>2.</td><td>Basic concepts of diffusion and convection</td><td>Convective and diffusive fluxes - Sec. 2.1.1 and 2.1.2 of V Kumaran Mass, heat, and momentum diffusion - Sec. 3.1 of V Kumaran</td><td></td></tr>
<tr><td>3</td><td>Steady and Unsteady unidirectional shell balance for Heat, Mass, and Linear momentum transport in Rectangular Coordinates</td><td>Governing conservation equations (Sec. 4.1 of VK) Steady heat conduction in single and multiple slabs (Sec. 4.2 of VK) Steady laminar flow down an inclined plane (Sec. 4.2 of VK) Steady diffusion with homogeneous reaction (Sec. 4.2 of VK) Unsteady transport into an infinite medium - similarity solution (Sec. 4.4 of VK) Steady diffusion into a falling liquid film (Sec. 4.4.1 of VK) Transient conduction in a slab of finite thickness - separation of variables solution (Sec. 4.7 of VK)</td><td>4</td></tr>
<tr><td>4</td><td>Steady and Unsteady unidirectional shell balance for Heat, Mass, and</td><td>Governing conservation equations in cylindrical coordinates (Sec. 5.1 of VK) Steady solutions for conduction/diffusion in</td><td>6</td></tr>
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<tr><td></td><td>Linear momentum transport in Curvilinear Coordinates</td><td>cylindrical coordinates (5.1.2 of VK) Heat conduction from a thin wire into an 6 infinite medium - similarity solution (5.1.3 of VK) Unsteady heat conduction into a cylinder - separation of variables solution (Sec. 5.1.4 of VK) Governing equations in spherical coordinates (5.2 of VK) Steady conduction from a spherical particle (5.2.2 of VK) Unsteady conduction in a sphere - separation of variables solution (5.2.3 of VK)</td><td></td></tr>
<tr><td>5</td><td>Forced convection, concept of Boundary Layers, Scaling analysis</td><td>Flow past a heated surface - derivation of Nusselt number - Peclet number correlation (9.1.1 of VK) Convective heat transfer due to flow around a solid particle (9.1.3 of VK) Convective heat transfer in flow past a mobile/fluid interface (9.2 of VK) 7</td><td>7</td></tr>
<tr><td colspan="3">Total</td><td>20</td></tr>
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<tr><td>CHE603M</td><td>Introduction to Thermodynamics</td><td></td><td>
The aim of this course is to introduce the key concepts of Chemical Engineering Thermodynamics to students with diverse backgrounds. Particularly, this course is useful for graduate students of allied branches who are interested in postgraduate programs in the chemical engineering department.
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<tr><th>S. No.</th><th>Broad Title</th><th>Topics</th><th>No.of Lectures</th></tr>
<tr><td>1</td><td>Introduction and First law</td><td>Heat, Work, conservation of mass and energy, Equilibrium state, intensive and extensive variables, Applications</td><td>2</td></tr>
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			2	**Second law and Entropy**	Entropy, Reversibility, Entropy changes of matter, Applications	**3**
			3	**Thermodynamic properties of real substances**	Corresponding states, Generalized equations of state, thermodynamic partial derivatives, thermodynamic property evaluations on change of state	**4**
			4	**Equilibrium in onecomponent systems**	Criterion for Equilibrium, Molar Gibbs energy and Fugacity of a pure component, Calculation of fluid-phase equilibrium – vapor pressure, Gibbs phase rule for one component system, Thermodynamic properties of phase transitions	**5**
			5	**Thermodynamics of multicomponent mixtures**	Partial molar properties, Gibbs Duhem equation, ideal solution and excess molar properties, Activity coefficients and models	**4**
			6	**Chemical Reaction Equilibrium**	Equilibrium in single phase system, homogeneous chemical reactions	**2**
CHE601M	Elementary Engineering Mathematics	3-0-0-0-(5)	The course will expose fresh PhD students to basic engineering mathematics to aid them in learning advanced courses in Chemical Engineering.			

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<tr><th>S. No.</th><th>Broad Title</th><th>Topics</th><th>No.of Lectures</th></tr>
<tr><td>1</td><td>Introductio to Multivariable Calculus</td><td>Functions of one or more variables, limits, chain rule of differentiation, change of variables, maxima/minima of function of two or more variables</td><td>3</td></tr>
<tr><td>2</td><td>Introduction to Multivariable Calculus</td><td>Complex numbers, Polar form, Powers and Roots, Logarithms</td><td>3</td></tr>
<tr><td>3</td><td>Linear Algebra</td><td>Matrices, vectors, determinants, solution of linear system of equations, eigenvalue problems</td><td>5</td></tr>
<tr><td>4</td><td>Ordinary Differential Equations</td><td>First order ODEs, second order linear ODEs</td><td>2</td></tr>
<tr><td>5</td><td>Fourier Analysis and PDEs</td><td>Fourier series, Fourier Transform, Laplace Transform, Classification of PDEs; PDE solution by separation of variables</td><td>7</td></tr>
<tr><td colspan="3">Total</td><td>20</td></tr>
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<td>CHE604M</td>
<td>Fundamentals of Chemical Reaction Engineering</td>
<td>3-0-0-0-(5)</td>
<td>
(A) Objectives: The course will expose fresh PhD students, especially those from allied disciplines, to the fundamentals of chemical reaction engineering. Taking this course is expected to assist the students in advanced courses related to chemical reaction engineering.
(B) Contents (preferably in the form of 5 to 10 broad titles):

<u>Lecture-wise break-up (considering the duration of each lecture is 50 minutes)</u>
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S. No.	Broad Title	Topics	No.of Lectures
1	Idealization in chemical reaction engineering	Basic definitions, Development of species mol balance and energy balance equations for idealized reactors	1
2	Steady & unsteady state operation in idealized reactors	Design equations for idealized batch and flow reactors (CSTR, PFR, PBR), Multiple reactors	3
3	Multiple reactions	Parallel, series and complex reactions in idealized reactors	2
4	Nonelementary reaction kinetics	Development of rate laws that do not follow power-law kinetics	3
5	Modelling of catalytic reaction kinetics	Analysis of reaction data from different idealized reactors, differential, integral, halflives, etc	3
6	External diffusion effects on heterogeneous reactions	Multiphase reactionsand effects of external diffusion; determination of concentration differences between surface and the bulk	2
7	Diffusion and reaction in porous catalysts	Internal mass transfer effects in porous catalysts under isothermal conditions, Thiele modulus, Effectiveness factor, Falsified kinetics	4
8	Design of fixed bed reactors	An example of an isothermal heterogeneously catalysed reaction with development of rate law, effect of change in mols and effect of pressure	2
Total			**20**

CHE657	Machine Learning in Chemical Engineering	3-0-0-0-(9)	**(A)Objectives:** This course will introduce students to machine learning (ML) applications across various areas of chemical engineering. Students will also be introduced to various ML Python libraries and most lectures will involve hands-on case studies. The course is particularly targeted towards postgraduate students and has been designed to help both, experimentalists and computational researchers. **(C) Contents (preferably in the form of 5 to 10 broad titles):** Lecture-wise break-up (considering the duration of each lecture is 50 minutes)

S. No.	Broad Title	Topics	No.of Lectures
1.	Basics of machine learning (ML) and its application to chemical engineering	Broad overview of ML and its application to various areas of chemical engineering. Introduction to Python and Python libraries to be used in the course.	**3**
2.	Data pre-processing for chemical engineering data	Introduction to different types of data in chemical engineering (molecular datasets and spatiotemporal data). Handling missing data and feature scaling. Introduction to the scikit-learn Python library.	**3**
3.	Dimensionality reduction techniques	Feature selection and linear dimensionality reduction (PCA, LDA). Non-linear dimensionality reduction (diffusion maps).	**3**
4.	Classification methods applied to chemical engineering data	Logistic regression, k-nearest neighbours, decision trees, and random forest. Introduction to the RDKIT python library for cheminformatics. Implementing	**3**

						classification methods for molecular data with RDKIT and scikit-learn	
				5.	Regression methods applied to chemical engineering data	Linear regression, polynomial regression, and lasso regression. Implementing regression methods with the scikit-learn Python library. Regression methods applied to predicting chemical properties from chemical/material structure (e.g. solubility, heat capacities etc.).	**4**
				6.	Neural networks and deep learning in chemical engineering	Multi-layer perceptron, activation functions, and backpropagation. Training neural networks with the PyTorch Python library. Modeling reactor dynamics with neural networks.	**3**
				7.	Physics informed neural networks (PINNs) for solving PDEs for chemical engineering problems	Introduction to PINNs and training PINNs with the PINA Python library. Solving reaction diffusion PDEs with PINNs.	**3**
				8.	Uncertainty quantification of ML predicted properties	Ensemble methods, Gini importance, and Bayesian optimization. Introduction to the PyStan Python library for Bayesian inference and its application to molecular properties predicted from structure.	**5**
				9.	Natural Language Processing (NLP) and Large language models (LLMs)	Introduction to NLP and LLMs. Application of LLMs to mining and	**3**

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<tr><td></td><td></td><td>organizing chemical data from unstructured data sources.</td><td></td></tr>
<tr><td>10.</td><td>Transfer learning and domain adaptation</td><td>Introduction to transfer learning and domain adaptation. Introduction to the ADAPT Python library applied to learn molecular properties with limited data</td><td>4</td></tr>
<tr><td>11.</td><td>Symbolic regression for discovering equations from data</td><td>Genetic programming for symbolic regression. Introduction to the gplearn Python package to discover symbolic expressions from thermodynamic data</td><td>3</td></tr>
<tr><td>12.</td><td>Material and chemical discovery with generative AI</td><td>Generative adversarial networks and variational autoencoders. Application of generative AI for material discovery.</td><td>3</td></tr>
<tr><td colspan="3">Total</td><td>40</td></tr>
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<tr><td>CHE627</td><td>Computational Methods in Chemical Engineering</td><td>2-0-3-0-9</td><td>The course is targeted for graduate-level students employing numerical and computational techniques for their research. The aim is to equip students with the theoretical foundations and practical exposure to these methods for solving complex problems in (chemical) engineering. The course is designed to have a combination of lectures and hands-on sessions using programming environments such as python (or matlab) aiming to develop skills to model, analyze, and address problems that are difficult to solve analytically; preparing them for advanced research and industrial challenges.</td></tr>
<tr><td>CHE624</td><td>An Introduction to Mathematical Medicine</td><td>3-0-0-0-9</td><td>(A) Objectives: Students taking this course will learn about a theoretical and mathematical understanding of various human diseases.

(B) Contents (preferably in the form of 5 to 10 broad titles):

1. Hormone circuits (4)

2. Dynamical compensation, mutant resistance, and type-2 diabetes (4)

3. The stress hormone axis as a two-gland oscillator (5)

4. The thyroid and its discontents (4)</td></tr>
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			5. Autoimmune diseases as a fragility of mutant surveillance (5) 6. Inflammation and fibrosis as a bistable system (4) 7. Basic facts of aging (4) 8. Aging and Saturated repair (5) 9. Age-related diseases (4) Total lectures: 39
CHE647	Linear and discrete optimization for process systems engineering	3-0-3-0 (12)	This course provides an introduction to linear and integer optimization. Students will learn how to formulate linear and mixed-integer optimization models for practical engineering applications and solve them using state-of-the-art solvers (e.g., Gurobi). The course also covers foundational theory and algorithms for solving these optimization problems. The course has several hands-on laboratory sessions to implement and solve optimization models using Python API of Gurobi. In addition, students will gain exposure to implementing selected optimization algorithms.
CHE653	Fundamentals of reservoir engineering	3-0-0-0 (9)	**Objectives**: Reservoir engineering involves understanding fluid flow in the subsurface porous media and optimizing the production of oil and gas from the subsurface. The same set of principles are also useful in gas storage applications including CO2 sequestration, hydrogen storage, etc. The objective of this course is to provide a fundamental understanding of fluid flow in porous media and reservoir engineering.
CHE648	CFD-Based Simulation of Transport Phenomena in Chemical Engineering	3-0-0-0 (9)	Transport Phenomena is one of the core subjects in Chemical Engineering and traditionally relies on analytical solutions of the governing equations of momentum, heat and mass transfer. While these classical solutions provide valuable physical insight, modern engineering practice increasingly employs Computational Fluid Dynamics (CFD) for analysing transport processes encountered in industrial equipment and processes. This course aims to complement the traditional analytical treatment of Transport Phenomena by introducing CFD as a learning and analysis tool. Students will simulate classical transport problems using ANSYS Fluent and compare the numerical predictions with available analytical or semi-analytical solutions. Emphasis will be placed on physical understanding of transport phenomena, model development, mesh generation, specification of boundary conditions, solution convergence, validation and interpretation of simulation results rather than on the mathematical formulation of CFD algorithms. Upon successful completion of the course, students will be able to: • Develop CFD models for classical Chemical Engineering transport problems. • Generate suitable computational meshes and prescribe appropriate boundary conditions. • Simulate momentum, heat and mass transfer using ANSYS Fluent. • Validate CFD predictions against analytical solutions and established correlations. • Critically interpret simulation results and apply CFD as an engineering tool for solving transport problems encountered in Chemical Engineering practice.