

CHEMICAL ENGINEERING

I Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits (AL/3)
CHE 101	Introduction to Engineering	2	0	3	0	0	5	2	S/X	2

III Semester:

	Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits (AL/3)
DC	CHE201	Engineering Mechanics (Solid & Fluid)	3	0	4.5	0	0	7.5	3	O to F	3
	CHE203	Introduction to Thermodynamics	3	0	4.5	0	0	7.5	3	O to F	3
MD	MTH201	Multivariable Calculus	3	1	4.5	0	0	8.5	4	O to F	3

IV Semester:

	Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits (AL/3)
Chemical Engineering											
DC	CHE202	Chemical Engineering Thermodynamics	3	0	4.5	0	0	7.5	3	O to F	3
	CHE204	Chemical Process Calculations	3	0	4.5	0	0	7.5	3	O to F	3
	CHE206	Introduction to Chemical Engineering Laboratory	0	0	1	3	0	4	3	O to F	1
MD	MTH202	Probability and Statistics	3	1	4.5	0	0	8.5	4	O to F	3

DC: Departmental Compulsory Course; **MD:** Mandatory Course from Other Department

V Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHE 301	Heat Transfer Operations	3	0	7.5	0	0	10.5	3	O to F	4
CHE 303	Fluid Mechanics and Mechanical Operations	3	0	7.5	0	0	10.5	3	O to F	4
CHE 305	Numerical Methods in Chemical Engineering	2	0	6	3	0	11	5	O to F	4
CHE 307	Thermodynamics Laboratory	0	0	1.5	4	0	5.5	4	O to F	2
CHE ***	Department Elective – I	3	0	7.5	0	0	10.5	3	O to F	4
*** **	Open Elective – I	3	0	7.5	0	0	10.5	3	O to F	4
Total Credits		14	0	37.5	7	0	58.5	21	-	22

VI Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHE 302	Chemical Reaction Engineering-I	3	0	7.5	0	0	10.5	3	O to F	4
CHE 304	Mass Transfer and Separation Process	3	0	7.5	0	0	10.5	3	O to F	4
CHE 306	Heat Transfer Laboratory	0	0	1.5	4	0	5.5	4	O to F	2
CHE 308	Fluid Mechanics Laboratory	0	0	1.5	4	0	5.5	4	O to F	2
CHE ***	Department Elective – II	3	0	7.5	0	0	10.5	3	O to F	4
*** **	Open Elective – II	3	0	7.5	0	0	10.5	3	O to F	4
Total Credits		12	0	36	8	0	53	20	-	20

VII Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHE 401/ 421	Statistical Mechanics	3	0	7.5	0	0	10.5	3	O to F	4
CHE 403	Process Dynamics and Control	3	0	7.5	0	0	10.5	3	O to F	4
CHE 407	Chemical Reaction Engineering Laboratory	0	0	1.5	4	0	5.5	4	O to F	2
CHE 409	Mass Transfer Laboratory	0	0	1.5	4	0	5.5	4	O to F	2
CHE ***	Department Elective – III	3	0	7.5	0	0	10.5	3	O to F	4
*** **	Open Elective – III	3	0	7.5	0	0	10.5	3	O to F	4
Total Credits		12	0	33	8	0	53	20	-	20

VIII Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHE 402	Process Design and Economics	3	0	7.5	0	0	10.5	3	O to F	4
CHE 404	Chemical Reaction Engineering-II	3	0	7.5	0	0	10.5	3	O to F	4
CHE 406	Advanced Transport Phenomena	3	0	7.5	0	0	10.5	3	O to F	4
CHE 408	Process Control and Instrumentation Laboratory	0	0	1.5	4	0	5.5	4	O to F	2
CHE ***	Department Elective – IV	3	0	7.5	0	0	10.5	3	O to F	4
*** **	Open Elective – IV	3	0	7.5	0	0	10.5	3	O to F	4
Total Credits		15	0	39	4	0	58	19	-	22

IX Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHE 501	MS Thesis	-	-	-	-	-	30	-	O to F	12
CHE ***	Department Elective – V	3	0	7.5	0	0	10.5	3	O to F	4
*** **	Open Elective – V	3	0	7.5	0	0	10.5	3	O to F	4
HSS 503	Law Relating to Intellectual Property and Patents	1	0	2.5	0	0	3.5	1	S/X	1
Total Credits		7	0	16.5	0	0	53.5	7	-	21

X Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHE 501	MS Thesis	-	-	-	-	-	45	-	O to F	18
Total Credits		-	-	-	-	-	45	-	-	18

CHE 101: Introduction to Engineering (2)

Learning Objectives

This course will expose the students to theoretical, computational and experimental aspects of engineering including technological evolution of products using case studies. It will also involve hands on assembling/ disassembling of engineering products to enable students to understand how scientific concepts are used to design a device/product.

Course Contents

Introduction to engineering: what is engineering, engineering design, disciplines of engineering etc.; Engineering tools, roles of engineers in society such as research & development, testing, designing, construction, analysis, technical support, management, consultancy etc.; demonstration of engineering principles using real life examples; hands on design for understanding the mechanism.

Introduction to Machine Learning, Robotics, Hands on with Arduino/ Raspberry Pi, Topics in Electromagnetism, Topics in Signal Processing, Topics in Devices & Circuits, Design and verification of safety critical systems, Topics in Algorithms

Papers

Note (If any): 1 hr/ 2 hrs of lecture and 3 hrs of lab per week. Assignments to be given at the end of each week. Final grade to be based on these assignments and attendance. Also, a ‘tinkering’ lab will be available to facilitate the achievement of course objectives.

CHE 201: Engineering Mechanics (3)

Learning Objectives

To expose the students to fundamentals of solid and fluid mechanics. At the end of the course, the students should be able to mathematically formulate and solve simple problems involving elastic deformation of solids, estimation of stresses, analyze elementary fluid flows and understand the working principle of flow measuring devices.

Course Contents

Part I (Solid Mechanics): Introduction to stress and strain: stress at a point, Cauchy stress tensor, analysis of deformation and definition of strain components, principal stresses and strains, stress and strain invariants, Mohr's circle representation, Shear force and bending moment diagrams, Axially loaded members, Torsion of circular shafts, Stresses due to bending: pure bending, transverse shear.

Part II (Fluid Mechanics): Basic concept of fluid properties and classification of fluids: statics of fluid, viscosity, surface tension, Newtonian and non-Newtonian fluids; Kinematics of fluid: concept of stress, rate of strain, streamlines, streak lines, path lines, stream function; Fluid motion and mathematical modelling: Navier-Stokes equation, Euler and Bernoulli equation; Dimensional analysis and dimensionless numbers, Flow measuring devices and their industrial applications: pitot tube, venturi meter, orifice meter, rotameter etc.; Pumps.

Text Books

1. R.C. Hibbeler, Mechanics of Materials, 8th Edition, Prentice Hall, 2011.
2. R.W. Fox, A.T. MacDonald and P.J. Pritchard, Introduction to Fluid Mechanics, Wiley, 2008

References

1. H. Shames and J. M. Pitarresi, Introduction to Solid Mechanics, Prentice Hall of India, 2003.
2. F.M. White, Fluid Mechanics, 7th Ed., McGraw Hill, 2009.
3. V. Gupta and S.K. Gupta, Fluid Mechanics and Its Applications, 3rd Ed., New Age Publishers, 2015.

CHE 202: Chemical Engineering Thermodynamics (3)

Learning Objectives

The purpose of this course is to understand thermodynamics from a Chemical Engineering point of view. At the end of this course, students should be able to estimate thermodynamic properties (such as activity coefficient, vapor-liquid compositions etc.) of reacting as well as non-reacting multi-phase, multi-component systems.

Course Contents

Laws of Thermodynamics: Introduction, Work, Heat, Energy , Review of first Law for closed and open systems, properties of ideal gas and real fluids

Reversibility and Entropy: Reversibility, the second law of thermodynamics, Carnot engine, entropy change for closed and open system

Fundamental Equations: Thermodynamics calculus, thermodynamics derivatives, Euler's theorem for homogeneous functions, Legendre's transformations, Derivative in terms of measurable properties

Microscopic origin of entropy and elementary statistical mechanics

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

Text books

1. Engineering and Chemical Thermodynamics, M. D. Koretsky, Wiley India, 2004.

References

1. S. I. Sandler, Chemical, Biochemical and Engineering Thermodynamics, Wiley, 2006

2. Smith, van Ness and Abbott, Chemical Engineering Thermodynamics, 7th Ed., McGraw-Hill, 2005
3. Y. V. Rao, Chemical Engineering Thermodynamics, Universities Press, India, 1997

CHE 203: Introduction to Thermodynamics (3)

Learning Objectives

The purpose of this course is to introduce basic thermodynamic concepts such as work, heat, internal energy, enthalpy, entropy. At the end of the course, the students should be able to apply the laws of thermodynamics to analyze heat engines, refrigerators etc.

Course Contents

Definitions & Concepts: System & CV, Macroscopic and microscopic view points; Property, Thermodynamic State & Equilibrium, Energy, Work interaction & various modes of work, Heat; Zeroth Law of Thermodynamics, Temperature Scale

Properties of Pure Substances: Pure substance, Phase, Simple compressible substance, Ideal gas Equation of State, van der Waals Equation of State; Law of corresponding states, Compressibility chart, Pressure- volume; Temperature-volume and Phase diagrams; Mollier diagram and Steam tables.

First Law of Thermodynamics & its consequences: First law for a control mass; Internal energy; I Law analysis of Non-flow processes; Use of steam tables & Mollier diagram, Application of I Law of Thermodynamics for Flow Process (CV) –Steady-state processes, Throttling process; Transient Flow Processes - Charging & discharging of tanks.

I Law Application to Chemically Reacting Systems: Fuels & Combustion, Theoretical Air/Fuel ratio, Standard heat of Reaction and effect of temperature on standard heat of reaction, Adiabatic flame temperature.

II Law of Thermodynamics & its Applications: Limitations of the I Law of Thermodynamics, Heat Engine, Heat Pump/Refrigerator. II Law of Thermodynamics – Kelvin Planck and Clausius statements & their equivalence. Reversible & irreversible processes, Criterion of reversibility, Carnot cycle &

Carnot principles, Thermodynamic Temperature scale, Clausius inequality, Entropy, Calculations of entropy change, Principle of entropy increase, T-S diagram, II Law analysis of Control Volume. Available energy, Availability; Second law efficiency

Thermodynamic Potentials: Maxwell relations, Thermodynamic relations, Jacobian methods, Clapeyron and Kirchoff equations, Phase rule.

Power Cycles: Rankine cycle – Ideal and Reheat. Gas Power Cycles; Otto cycle, Diesel cycle and Brayton cycle.

Refrigeration Cycles: Vapor compression cycle, Air-standard refrigeration cycle.

Text Books:

1. C. Borgnakke and R. E. Sonntag, Fundamentals of Thermodynamics, 7th Ed., Wiley, 2009.
2. Cengel and Boles, Thermodynamics An Engineering Approach, 6th Ed., Tata McGraw Hill, 2008.

CHE 204: Chemical Process Calculation (3)

Learning Objectives

At the end of the course students should be to apply the principles of mass and energy balances for solving steady and unsteady state problems for reacting and non-reacting chemical processes.

Course Contents

Objectives and overview: Historical perspective and chemical engineering, role of a chemical engineer, Role of balance, Calculations, Review of basic concepts

Steady state –material balance in non-reacting system: On single units, Basis of calculation, Number of independent equations, development of degrees of freedom, specification of variables. Balance on multiple unit processes: recycle and bypass

Balances in Reacting systems: Stoichiometry, multiple reactions, recycle and purge

Element (Atomic) versus species (molecular balance): Combustion of fossil

fuels, ultimate (elemental) and approximate analyses, combustion chemistry-incomplete combustion, theoretical and excess air

Material balances in multiphase systems: Phase rule, gas-liquid system, vapor-liquid equilibrium (VLE) calculation, isothermal flash vaporization, immiscible and partially miscible liquid system, solid-liquid systems; saturation solubility and crystallization

General energy balance: steady-state energy in non-reacting system, heat capacity, enthalpy (and internal energy) changes from heat capacity equations, balances involving phase changes and mixing, effect of temperature on enthalpy of phase change

Energy balances in reacting system: standard heat of reaction, heats of formation and combustion. Fuels and combustion: higher (gross) and lower (net) heating values, adiabatic (theoretical) flame temperature

Psychrometry: Basic definitions, use of psychrometric chart-properties of moist air, enthalpy changes, adiabatic humidification and dehumidification calculation

Unsteady-state material and energy balance: tank hold-up and discharge, batch reactor, batch distillation, Energy balances (single-phase, non-reacting systems): startup of a reactor, heat loss from a storage tank.

Text books

Elementary Principles of Chemical Processes, R. M. Felder and R. W. Rousseau.

Reference:

David M. Himmelblau, Basic Principles and Calculation in Chemical Engineering, 8th Ed., PHI, 2016

B. I. Bhatt and S. B. Thakore, Stoichiometry, Tata McGraw Hill, 2010.

CHE 301: Heat Transfer Operations (4)

Learning Objectives

At the end of this course, the students should understand the laws governing the different modes of heat transfer and apply these to the design of heat transfer equipment.

Course Contents

Basic modes of heat transfer,

Conduction: principles and basic equations of 1D, 2D and 3D conduction, Fourier's law, steady state heat transfer through composite slabs, composite cylinders and sphere; Critical thickness of insulation, Fin effectiveness and efficiency, Lumped parameter approach and significance of time constant.

Convection: natural and forced convection, hydrodynamic and thermal boundary layers, Individual

& overall heat transfer coefficient, log-mean temperature difference (LMTD), Empirical equations for free and forced convection,

Types of heat exchangers and related problem in industries, LMTD method, effectiveness-NTU method;

Radiation: black body and gray body radiation, Laws of black body radiation, Evaporation: basic concepts of vaporization, single & multiple effect evaporators.

Textbook

1. B.K. Dutta, Heat Transfer, Prentice Hall of India, 2001.

References

1. J.P. Holman, Heat Transfer, 8th Ed., McGraw - Hill, 1997.
2. D.Q. Kern, Process Heat Transfer, 2nd Ed., Tata McGraw - Hill, 1997

CHE 302: Chemical Reaction Engineering-I (4)

Learning Objectives

At the end of the course, students should be able to determine the kinetics of elementary and non- elementary homogeneous reactions and apply these for design of different types of reactors.

Course Contents

Introduction: definition of rate of reaction; general mole balance equation; design equations for ideal reactors;

Application of design equations to batch and flow systems; reactors in series;

Basic concepts in chemical kinetics; relationship of concentration of limiting; conversion in constant volume and variable volume systems

Design of isothermal ideal reactors for simple irreversible and reversible reactions; recycle reactors; unsteady state operation of reactors; simultaneous; reaction and separation;

Determination of reaction rate expressions from experimental data – differential and integral method of analysis, method of initial rates, method of half-lives; least-square analysis;

Non-elementary homogeneous reactions; determination of rate expression from reaction mechanism; chain reactions; reactions involving enzymes;

Non-isothermal reactor design – the energy balance, design of non-isothermal CSTR and PFR. Unsteady state operation – CSTR, PFR and batch reactor. Multiple steady states in a CSTR; Multiple reactions in ideal reactors;

Analysis of non-ideal reactors – residence time distribution; zero-parameter models – segregated flow and maximum mixedness models; one-parameter models-tank-in-series model and dispersion model.

Scale-up of chemical reactors.

Textbook

1. H. S. Fogler, Elements of Chemical Reaction Engineering, 4th Ed., Prentice-Hall of India, New Delhi, 2009.

References

1. O. Levenspiel, Chemical Reaction Engineering, 3rd Ed, Wiley-Eastern Ltd., 1999
2. J.M. Smith, Chemical Engineering Kinetics, 3rd Ed., McGraw-Hill, 1981

CHE 303: Fluid Mechanics and Mechanical Operations (4)

Learning Objectives

At the end of this course, students should be able to apply the principles of fluid mechanics to estimate pressure drop in pipe flows, packed beds, fluidized beds, and estimate drag forces in flow past solid objects. The students will also understand the principles of scale-up and apply it to various chemical

engineering equipment involving fluid flow such as pumps, settling tanks, and cyclones.

Course Contents

Differential balance: differential equation of mass conservation, differential equation of linear momentum, constitutive equations, Navier-stokes equations

Applications to Couette flow between a fixed and a moving plate, flow due to pressure gradient between two fixed plates, fully developed laminar pipe flow-Hagen-Poiseuille flow, pipe flow with a power law fluid

Dimensional analysis and similarity: Buckingham Pi-theorem, non-dimensionalization of continuity and Navier-Stokes equations, introduction of dimensionless numbers

Pipe/Duct flows: laminar vs turbulent flows, kinetic energy correction factor (α), momentum flux correction factor (β), head loss, friction factor, effect of wall roughness, the Moody chart, hydraulic diameter for non-circular conduit, minor losses (entrances/exits, expansion/contraction, fittings and valves), equivalent length

Flow meters: Pitot tubes, venturi, orifice, rotameter, introduction to non-invasive flow measurement techniques

Flow past immersed bodies: creeping flow-Stokes law, inviscid flow-Bernoulli equation, introduction to boundary layer, Karman's momentum integral theory, drag on flat plate for laminar flow, drag on immersed bodies- C_D vs. Re plot

Flow through packed and fluidized beds: Flow through beds of solids, motion of particles through the fluid, Kozeny-Carman equations, Ergun equation, Fluidization, minimum fluidization velocity. Particle settling

Centrifuges and cyclones: gravity settling, centrifugal separation, design of cyclones

Mixing and agitation: types of impeller, flow no., power consumption, mixing times, scale up

Flow machinery: Introduction to pump, performance curve of a centrifugal pump, efficiency, priming, cavitation and NPSH, introduction to fans, blowers and compressor

Size Reduction of solids: Crushing, Grinding, Mechanism of size reduction.

Textbook

1. R.W. Fox, A.T. MacDonald and P.J. Pritchard, Introduction to Fluid Mechanics Wiley, 2008.

References

1. W.L. McCabe, J. Smith and P. Harriot, Unit Operations of Chemical Engineering, 6th Ed., McGraw - Hill, International Edition, 2001.
2. J.O. Wilkes, Fluid Mechanics for chemical engineers with microfluidics and CFD, 2nd ed., Prentice Hall, 1998.
3. M. Denn, Process Fluid Mechanics, Prentice Hall, 1979.
4. R. S. Hiremath and A.. P. Kulkarni, Mechanical Operations Vol.-I.

CHE 304: Mass Transfer and Separation Process (4)

Learning Objectives

At the end of the course, the student will be able to apply the principles of diffusive and convective mass transfer both in single and multi-phase systems. The students will be able to design equipment for separation processes such as gas absorption, distillation, extraction, and adsorption.

Course Contents

Mass transfer related unit operations in process industries: absorption, distillation, liquid-liquid extraction, adsorption; Design and performance of unit operations: rate and equilibrium stage based modeling approaches.

Fundamentals of mass transfer, Fick's law, mass transfer coefficients, unsteady state diffusion (analogy with heat transfer), film theory/surface renewal theory/boundary layer theory, species continuity balance, interphase mass transfer,

Continuous contactors: material balance and operating line, co-current and counter-current continuous processes;

Mass transfer equipment: Sparged vessels, agitated vessels, tray columns and packed columns; mass transfer coefficients for packed columns

Review of phase equilibria: gas-liquid, liquid-liquid, vapour-liquid and gas-solid

Absorption: Equilibrium approach: material balance, operating line, minimum liquid flow rates, number of equilibrium stages, deviation from ideal systems (stage and Murphee efficiency) Rate approach: Number of transfer units (NTU), height of transfer units (HTU) Packed and staged columns, hydrodynamic considerations: loading and flooding criterion, pressure-drops

Distillation: Flash distillation, Ponchon-Savarit and McCabe-Thiele methods for equilibrium stage calculations, Minimum and total reflux, optimum design, deviation from ideal system, azeotropic distillation (only introduction)

Extraction: Single-stage and multistage extraction

Adsorption and chromatography: Single-stage, multi-stage cross-current operations, packed-bed continuous contactor, breakthrough curves, rate equations for non-porous and porous adsorbents

Humidification and Drying: Dry and wet bulb temperatures, humidity, relative and percentage humidity, psychrometry chart, and adiabatic saturation temperature; Equilibrium, drying rate curve, rate and time of batch drying, mechanisms of batch drying, continuous drying

Textbook

1. B.K. Dutta, Principles of Mass Transfer and Separation Processes, 1st Ed., Prentice Hall of India, 2007.

References

1. R.E. Treybal, Mass Transfer Operations, 3rd Ed, McGraw Hill Education, 2012
2. J.D. Seader and E.J. Henley, Separation Process Principles, 2nd ed., Wiley, 2005.
3. E.L. Cussler, Diffusion: Mass Transfer in Fluid Systems, 2nd ed., Cambridge series, 1997.
4. W.L. McCabe, J. Smith and P. Harriot, Unit Operations of Chemical Engineering, 6th Ed., McGraw- Hill, International Edition, 2001.
5. D. M. Ruthven, Principles of adsorption and adsorption processes, John Wiley & sons, 1984
6. S. Sourirajan and T. Matsura, Reverse Osmosis and Ultrafiltration Process Principles, NRC Publication, Ottawa, 1985
7. J. G. S. Marcano and T. T. Tsotsis, Catalytic membranes and membrane

reactor, John Wiley, 2002

8. M.A. McHugh and V. J. Krukonis, Supercritical fluid extraction, Butterworths, Boston, 1985

CHE 305: Numerical Methods in Chemical Engineering (4)

Learning Objectives

The student will be able to apply a suite of numerical methods to develop computer codes (e.g. using Matlab) to solve a wide class of problems that are encountered in chemical engineering such as systems of linear and non-linear equations, ordinary and partial differential equations, numerical integration, function approximation etc.

Course Contents

Solution of linear algebraic equations - Gauss elimination, Gauss Jordan, Gauss Siedel; nonlinear algebraic equations - Newton Raphson(single and multiple equations); Linear and nonlinear regression; Approximation of functions (Newton's interpolation, Lagrange interpolation, orthogonal polynomials, cubic spline) Numerical integration(trapezoidal rule, Simpson's rule, quadrature methods); Solution of ordinary differential equations - IVPs (Euler, implicit Euler, Runge-Kutta) and Solution of ordinary differential equations - BVPs (finite difference, orthogonal collocation); Solution of partial differential equations (finite difference).

Textbook

1. S. K. Gupta, Numerical methods for engineers, New Age International, 2001.

Reference

1. S. C. Chapra and R. P. Canale, Numerical methods for engineers, Tata McGraw Hill, 2002

CHE 401/CHM421: Statistical Mechanics (4)

Learning Objectives

Statistical mechanics is a theoretical framework that allows establishing a bridge between the microscopic world and the behavior of macroscopic material which is amenable to experiment. The main objective of this course is to develop an understanding of the statistical nature of the laws of thermodynamics and calculate the physical properties of systems starting from the interactions between the constituent particles. We will discuss the basic principles of statistical mechanics and its applications to various physical and chemical processes in many-body systems.

Course Contents

Review of classical thermodynamics: Laws of thermodynamics and thermodynamic potentials, Legendre transforms and derivative relations, conditions of thermodynamic equilibrium and stability.

Elementary probability theory: Definition of probability, distribution functions and moments, average, variance and binomial distribution for large numbers and central limit theorem, statistical concept of uncertainty.

Fundamental principles of statistical mechanics: Macroscopic and microscopic states, fundamental postulates of statistical mechanics, statistical mechanical ensembles and their distribution functions, partition functions, entropy and Boltzmann distribution law, relation between partition functions and thermodynamic quantities in different ensembles, and fluctuations.

Ideal systems: Monatomic, diatomic and polyatomic gases and calculation of partition functions, heat capacities of gases, equipartition theorem and the Maxwell velocity distribution, Gibbs paradox, ortho- and para-hydrogen, blackbody radiation, heat capacities of solids (Einstein and Debye models), chemical equilibrium in ideal gas mixtures, photon and phonon gas systems of quantum particles and concept of different populations (Bose-Einstein and Fermi-Dirac statistics), distribution function of ideal Bose and Fermi gases, classical limits of quantum systems.

Suggested Book

1. H.B. Callen, Thermodynamics and an Introduction to Thermostatistics, 2nd Ed., Wiley, 1985.

2. T. L. Hill, An Introduction to Statistical Thermodynamics, Dover, 1987.
3. D.A. McQuarrie, Statistical Mechanics, University Science Books, 2000.
4. B. Widom, Statistical Mechanics: A Concise Introduction for Chemists, Cambridge University Press, 2002.
5. D. Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press, 1987.
6. R.K. Pathria,, Statistical Mechanics, Ed. 2nd, Butterworth-Heinemann, 1996.

CHE 402: Process Design and Economics (4)

Learning Objectives

The student will be able to synthesize concepts learnt in various unit operations to optimally design a process for producing a desired product. The student will also learn the optimal use of energy and materials in the design. The student will also be able to estimate the cost and profitability of the process.

Course Contents

Process Economics - Plant and equipment cost estimation, time value of money, profitability measures, taxes, depreciation.

Conceptual Process Synthesis - Systematic hierarchical synthesis of a flow sheet, structural layers of a flow sheet.

Reactor Network Synthesis - Choosing type of reactor and operating conditions for simple reaction systems, use of attainable region diagrams for complex reaction systems.

Separation system synthesis - Distillation column sequencing for ideal liquid mixtures, residue curve maps and their use in separation system design for non-ideal mixtures

Heat Exchanger Network Synthesis using Pinch technology - Targets for minimum utilities, area, total cost. Maximum Energy Recovery design, Evolutionary synthesis, Super-targeting, Heat and Power Integration

Textbook

1. R. Smith, Chemical Process Design and Integration, John Wiley & Sons, 2005

References

1. Seider, W.D., Seader, J.D., Lewin, D.R., Product and Process Design Principles, John Wiley & Sons, 2nd Ed., 2004
2. M.S. Peters and K.D. Timmerhaus, Plant Design and Economics for Chemical Engineers, McGraw Hill, 2003
3. D.F. Rudd and C.C. Watson, Strategy of Process Engineering, John Wiley, 1969

CHE 403: Process Dynamics and Control (4)

Learning Objectives

The student will be able to formulate mathematical models for describing the process dynamics and use them in the design of stable feed-back control loops (analog/digital) to achieve desired process performance. The students will be introduced to various measurement devices that constitute a control system.

Course Contents

Introduction to process control; Laplace transforms,

Types of models (continuous time domain, Laplace domain); Development of simple process models from first principles; Development of models from data,

Dynamical behaviour of first and second order systems: effect of poles, zeros and time delays on system response;

Introduction to feedback control: objectives, PID control; analysis of closed loop systems: stability, root locus, frequency response using Bode and Nyquist plots; control design techniques: design criteria, time and frequency domain techniques, model based design, tuning;

Advanced control strategies: cascade and feed forward, introduction to multivariable control;

Digital control: discrete time models, Z transform,

Instrumentation: measurement of pressure, temperature, flow and level; analog to digital conversion.

Textbook

1. D.E. Seborg, T.F. Edgar, D. A. Mellichamp, Process Dynamics and Control, John Wiley and Sons, 2nd ed., 2004.

References

1. G. Stephanopoulos, Chemical Process Control: An Introduction to Theory and Practice, Prentice Hall, New Jersey, 1984.
2. D. R. Coughanowr, and L. B. Koppel, Process systems Analysis and Control, 2nd Ed., McGrawHill, 1991.
3. W. L. Luyben, Process Modelling Simulation and Control for Chemical Engineers, McGraw Hill, 1990

CHE 404: Chemical Reaction Engineering – II (4)

Learning Objectives

The student will learn the principles behind the preparation and characterization of solid catalysts. The student will be able to develop kinetics for catalytic and non-catalytic heterogeneous reactions, and use these for the design of two-phase and multi-phase reactors.

Course Contents

Behaviour of chemical reactors - Mass, energy and momentum balance equations, batch reactor, PFR, CSTR, stability of CSTR.

Preparation and characterization of solid catalysts Catalysis - physical adsorption, chemisorption

Modelling of fluid-solid catalytic reactions - Langmuir-Hinshelwood models, redox kinetics, Mars-Krevlen kinetics

Diffusion and Reaction in Porous Catalysis - effective diffusivity, effectiveness factor, falsified kinetics, Intrapphase heat transfer effect - Praeter number, non-isothermal effectiveness factor Interphase heat and mass transfer effects in heterogeneous catalysts - global rate of reaction, overall effectiveness factor

Design of fixed bed reactors - 1D and 2D models, axial dispersion model

Catalyst deactivation - phenomena of catalyst deactivation (poisoning, fouling,

sintering), kinetics of catalyst deactivation, diffusional effects during catalyst deactivation

Gas-liquid reactions - review of physical mass transfer, different regimes of mass transfer with chemical reactions, general theory of mass transfer with chemical reactions, different types of gas- liquid reactors

Design of multiphase reactors - Types of multiphase reactors and their applications, determination of global rate for multiphase reactions, mechanical agitated slurry reactors, bubble column reactors, trickle bed reactor.

Fluid-solid non-catalytic reactions - shrinking core model, progressive reaction model, modelling of fluidized bed reactors (Kunii-Levenspiel model).

Textbook

1. G.F. Froment and K.B. Bischoff, Chemical Reactor Analysis and Design, John Wiley & Sons, N.Y., 1990.

References

1. H.S. Fogler, Elements of Chemical Reaction Engineering, Prentice-Hall, 3rd edition.
2. J.M. Smith, Chemical Engineering Kinetics, McGraw-Hill, International Student Edition (3rd Ed.).
3. J.J. Carberry, Chemical and Catalytic Reaction Engineering, McGraw-Hill, 1976.

CHE 406: Advanced Transport Phenomena (4)

Learning Objectives

The student will be able to apply the principles of fluid flow and transport to mathematically formulate and solve a variety of problems of interest in chemical engineering. The student will also be trained in making rational approximations to simplify the governing equations, and apply perturbation and asymptotic methods to obtain the solution.

Course Contents

Kinematics, Reynolds Transport theorem, Balance equations of momentum, energy and mass, Continuity equation for multi-component systems,

Constitutive relations,

Steady and unsteady solutions in rectilinear, cylindrical and spherical coordinates,

Approximation techniques and perturbation methods, Lubrication theory, Stream function, Creeping flows, Potential flow, Boundary layer theory (momentum and heat),

Turbulence; Inter-phase transport of momentum, energy and mass and macroscopic balances.

Textbook

1. W. Deen, Analysis of transport phenomena
2. L. G. Leal, Laminar Flow and Convective Transport Processes, Butterworth-Heinemann, 1992.