Proposed Course Structure and Syllabus for B.Tech. Chemical Engineering at IIT Patna

First Semester:

Subject ID	Subject	L-T-P	Credits
CE111	Engineering Drawing	1-0-3	5
EE101	Electrical Sciences	3-1-0	8
HS103	Communicative English for Engineers	2-0.5-1	6
MA101	Mathematics – I	3-1-0	8
ME110	Workshop-I	0-0-3	3
PH101	Physics – I	3-1-0	8
PH110	Physics Laboratory	0-0-3	3
	Sub-Total	12-3.5-10	**41**

Second Semester:

Subject ID	Subject	L-T-P	Credits
CB102 and CE102	Biology and Environmental Studies	3-0-0	6
CH101	Introductory Chemistry	3-1-0	8
CH110	Chemistry Laboratory	0-0-3	3
CS102	Programming and Data Structures	3-0-0	6
CS112	Programming and Data Structures Laboratory	0-0-3	3
EE102	Basic Electronics Laboratory	0-0-3	3
MA102	Mathematics – II	3-1-0	8
ME102	Engineering Mechanics	3-1-0	8
	Sub-Total	15-3-9	**45**

Third Semester:

Subject ID	Subject	L-T-P	Credits
MA201	Mathematics – III	3-1-0	8
CB211	Chemical Process Calculations	3-1-0	8
CB203	Fluid Mechanics	3-1-0	8
CB205	Mechanical Operations	3-0-0	6
HS2XX	HSS Elective – I	3-0-0	6
	Sub-Total	15-3-0	**36**

Fourth Semester:

Subject ID	Subject	L-T-P	Credits
CB202	Heat Transfer	3-1-0	8
CB204	Mass Transfer - I	2-1-0	6
CB206	Chemical Engineering Thermodynamics	3-0-0	6
CB208	Process Equipment Design - I	1-0-3	5
CB210	Mechanical Operations and Fluid Flow Lab	0-0-3	3
XX2nn	Open Elective-I	3-0-0	6
HS4XX	HSS Elective – II	3-0-0	6
	Sub-Total	15-2-6	**40**

Fifth Semester:

Subject ID	Subject	L-T-P	Credits
CB301	Chemical Reaction Engineering	2-1-0	6
CB303	Mass Transfer - II	2-1-0	6
CB305	Chemical Process Technology	3-0-0	6
CB307	Process Equipment Design - II	1-0-3	5
CB309	Mass Transfer Lab	0-0-3	3
CB317	Heat Transfer and Thermodynamics Lab	0-0-3	3
XX3nn	Open Elective-II	3-0-0	6
	Sub-Total	11-2-9	**35**

Sixth Semester:

Subject ID	Subject	L-T-P	Credits
CB318	Chemical Reactor Design	3-0-0	6
CB304	Chemical Process Modelling and Simulation	3-0-0	6
CB3XX	Departmental Elective -I	3-0-0	6
CB306	Chemical Process Simulation Lab	0-0-3	3
CB308	Process Control and Instrumentation	3-1-0	8
CB310	Chemical Reaction Engineering and Environmental Engineering Lab	0-0-3	3
HS3XX	HSS Elective – III	3-0-0	6
	Sub-Total	15-1-6	**38**

Seventh Semester:

Subject ID	Subject	L-T-P	Credits
CB401	Transport Phenomena	3-1-0	8
CB403	Summer Training	0-0-0	1
CB405	Process Control Lab	0-0-3	3
XX4nn	Open Elective – III	3-0-0	6
CB407	Process Plant Design and Economics	3-0-0	6
CB409	Grand Viva	0-0-0	1
CB417	Project-I	0-0-8	8
	Sub-Total	9-1-11	**33**

Eighth Semester:

Subject ID	Subject	L-T-P	Credits
CB4XX	Departmental Elective - II	3-0-0	6
CB4XX	Departmental Elective- III	3-0-0	6
CB4XX	Departmental Elective- IV	3-0-0	6
CB402	Project-II	0-0-12	12
	Sub-Total	9-0-12	**30**

Total Credit: 298 (at Par With Most of the IIT Systems)
Complied with Kakodkar Committee Report

Program Started from July 2016 with BOG Approval on 08.04.2016.

CB201   Chemical Process Calculations   LTPC 3-1-0-8

Pre-Requisites: None

Steady-state and dynamic processes; lumped and distributed processes; single and multi-phase systems; correlations for physical and transport properties; equilibrium relations; ideal gases and gaseous mixtures; vapor pressure; Vapor liquid equilibrium; Various Thermodynamics cycle such as Rankine Cycle, Carnot Cycle; Otto Cycle; Brayton Cycle; Material balances: non-reacting single-phase systems; systems with recycle, bypass and purge; processes involving vaporization and condensation. Intensive and extensive variables; rate laws; calculation of enthalpy change; heat of reaction; fuel calculations; saturation humidity, humidity charts and their use; energy balance calculations; flow-sheeting; degrees of freedom and its importance in flow-sheeting.

Text Books:

1. O. A. Hougen, K. M. Watson and R. A. Ragatz, *Chemical Process Principles, Part-I*, 2nd Ed., CBS Publishers, 2004
2. D. M. Himmelblau, *Basic Principles and Calculations in Chemical Engineering*, 8th Ed., Prentice Hall of India, 2014
3. R. M. Felder and R. W.Rousseau, *Elementary Principles of Chemical Processes*, 3rd Ed., Wiley, 2014
4. P. K. Nag, *Engineering Thermodynamics*, 5th Ed., Tata Mc-Graw Hill Education, 2013

Reference Books:

1. N. Chopey, *Handbook of Chemical Engineering Calculations*, 3rd Ed., Mc-Graw Hill, 2004

Pre-Requisites: None

Introduction, Types of fluids, Non-Newtonian viscosity, Dimensional Analysis (Buckingham PI theorem), Fluid statics, Hydrostatic force on submerged bodies, Rigid body motion, Kinematics of flow - Eulerian and Lagrangian descriptions, Integral analysis - mass and momentum balances, Bernoulli equation, Differential analysis of flow, Conservation of mass, linear and angular momentum, Navier-Stokes equation, Unidirectional flow, Viscous flow, Turbulent flow, Skin friction and form friction, Friction factor, Flow through pipes and ducts, Potential flow, Boundary layer theory, Boundary layer separation, Flow around immersed bodies, Drag & Lift, Flow through Packed and Fluidized Beds, Compressible flow, Flow measurement, Fluid transportation - pumps, blowers and compressors.

Text Books:

1. W. L. McCabe, J. C. Smith, P. Harriott, *Unit Operations of Chemical Engineering*, 7th Ed., Mc-Graw Hill, 2005

2. R. W. Fox, A. T. McDonald, P. J. Pritchard, *Introduction to Fluid Mechanics,* 7th Ed., Wiley, 2009

3. V. Gupta and S. K. Gupta, *Fluid Mechanics and its Applications*, 3rd Ed., New Academic Science Ltd, 2012

Reference Books:

1. M. Denn, *Process Fluid Mechanics*, Prentice Hall, 1979

2. V. L. Streeter, *Fluid Mechanics*, 5th Ed., Mc-Graw Hill, 1971

3. R. B. Bird, W. E. Stewart and E. N. Lightfoot, *Transport Phenomena*, 2nd Ed., Wiley, 2006

Prerequisite – None

Principles of crushing and grinding, Laws of crushing and grinding.Determination of mean particle size, Size distribution equations. Characteristics of industrial crushers and mills.Industrial screening, effectiveness of screens, cyclones. Fluid-particle mechanics, free and hindered settling. Industrial classifiers, clarifiers and thickeners, gravity separation, tabling and jigging. Floatation and its kinetics. Mixing of liquids and solids, power requirement in mixing. Principles of filtration, filtration equipment.

Text Books:

1. W. L. McCabe, J. C. Smith and P. Harriott, *Unit Operations of Chemical Engineering*, 7th Ed., Mc-Graw Hill, 2005
2. J. M. Coulson, J. F. Richardson, J. R. Backhurst and J. H. Harker, *Chemical Engineering*, Vol-2, 5th Ed., Elsevier, 2015

Reference Books:

1. A. M. Gaudin, *Principles of Mineral dressing*, Mc-Graw Hill, 1939
2. R. H. Perry and C. H. Chilton, *Chemical Engineers Hand Book*, 8th Ed., Mc-Graw Hill, 2007
3. A. F. Taggart, *Handbook of Mineral Dressing: Ores and Industrial Minerals*, Wiley, 1945

Prerequisite – None

INTRODUCTION – Typical heat transfer situations, Modes of heat transfer, Introduction to laws.

CONDUCTION – Fourier's law and thermal conductivity, Differential equation of heat conduction, boundary conditions and initial conditions, one dimensional steady state situations – plane wall, cylinder, sphere (simple and complex situations), concept of thermal resistance, critical radius, heat generation, pin fins, Two dimensional steady state situations, transient conduction, Lumped capacitance model, Heisler charts, Numerical methods in conduction, Steady state one dimensional and two dimensional problems.

RADIATION – Basic ideas, spectrum, basic definitions, Laws of radiation, black body radiation, Planck's law, Stefan Boltzman law, Wien's Displacement law, Lambert cosine law, Radiation exchange between black surfaces, shape factor, Radiation exchange between gray surfaces, radiosity-Irradiation method, Parallel plates.

FORCED CONVECTION –Concepts of fluid mechanics, Differential equation of heat convection, Laminar flow heat transfer in circular pipe – constant heat flux and constant wall temperature, thermal entrance region, Turbulent flow heat transfer in circular pipe, pipes of other cross sections, Heat transfer in laminar flow and turbulent flow over a flat plate, Reynolds analogy, Flow across a cylinder and sphere, flow across banks of tubes, impinging jets

NATURAL CONVECTION – Introduction, governing equations, Vertical plate - Pohlhausen solution, horizontal cylinder, horizontal plate, enclosed spaces

HEAT EXCHANGERS – Types of heat exchangers, LMTD approach – parallel, counter-flow, multi-pass and cross flow heat exchanger, NTU approach – parallel, counter-flow, shell and tube, cross-flow heat exchanger

CONDENSATION AND BOILING – Dimensionless parameters, boiling modes, correlations, forced convection boiling, laminar film condensation on a vertical plate, turbulent film condensation

Text Books:

1. D. Q. Kern, *Process Heat Transfer*, 1st Ed., Mc-Graw Hill, 2001
2. S. P. Sukhatme, *A Text Book of Heat Transfer*, 4th Ed., Universities press, 2005
3. J. P. Holman, *Heat Transfer*, 8th Ed., Mc-Graw Hill, 1996
1. W. L. McCabe, J. C. Smith and P. Harriott, *Unit Operations of Chemical Engineering*, 7th Ed., Mc-Graw Hill, 2005
2. G. G. Brown, *Unit Operations*, 1st Ed., CBS, 2005
3. W. H. McAdams, *Heat Transmission*, 2nd revised Ed., Mc-Graw Hill, 1973
4. H. Martin, *Heat exchangers*, 1st Ed., CRC press, 1988

Pre-requisites: None

Diffusion: Molecular Diffusion, Fick's law, Gas-Phase Diffusion Coefficient.

Convective Mass Transfer: Mass Transfer Coefficient - types, correlations; Eddy Diffusion; Theories of Mass Transfer. Inter-phase Mass Transfer: Equilibrium; Raoult's and Henry's Law; Mass Transfer between Two Phases; The Overall Mass Transfer Coefficient. Gas-Liquid Contacting Equipment: Introduction; Types – Tray or Plate, Agitated Vessel, Bubble Column, Packed Column, Spray tower etc.; Flooding in a Packed Tower. Gas Absorption and Stripping: Equilibrium in gas-Liquid Systems; Selection of Solvent; Design of Packed Tower; Correlations for Mass Transfer Coefficient; Determination of Number of Stages in Tray Tower; HETP. Distillation: Vapor-Liquid Equilibrium; Enthalpy-Concentration Diagram; Flash Vaporization;

Steam Distillation; Batch Distillation; Continuous Multistage Fractionation; McCabe-Thiele Method; Ponchon-Savarit Method. Liquid-Liquid Extraction: Liquid-Liquid Equilibrium; Examples of Solvent Extraction; Solvent Selection; Design Calculations. Solid-Liquid Extraction/Leaching: Rate, Solid-Liquid Contacting – Strategy, Equilibrium, Equipment; Calculations.

Text Books:

1. R. E. Treybal, *Mass Transfer Operations*, 3rd Ed., McGraw Hill, 1983

2. B. K. Dutta, *Principles of Mass Transfer and Separation Processes*, 8th Printing, PHI Learning Private Limited, 2015

Reference Books:

1. A. S. Foust, *Principles of Unit Operations*, 2nd Ed., Wiley, 1980

2. C.J. Geankoplis, *Transport Processes and Unit Operations*, 3rd Ed., Prentice Hall India, 1993

Pre-Requisites: None.

Introductory Concepts of Thermodynamic Systems and variables, Work, Heat, Internal Energy, Thermodynamic Equilibrium, Reversible and Irreversible Processes; PhaseRule; Significance of Chemical Engineering Thermodynamics; Equations of State and Generalized Correlations for Prediction of Volumetric Properties of Fluids; First Law: Closed and Open Systems, Steady and Transient Flow Processes; Second law and Entropy; Entropy Balance and Availability, Isentropic Efficiency; Maxwell Relations and Fluid Properties Estimation, Application to Flow Processes; Single Phase Mixtures and Solutions; Ideal Solutions; Partial molar quantities; Gibbs-Duhem Equation; Criteria for Thermodynamic Equilibrium; Phase Equilibrium Criteria, Non- ideal Solutions; Residual and Excess Properties; Fugacity and Activity Coefficient models; Pure Component Phase Equilibria, Vapour-Liquid Equilibria (VLE), Raoult's Law and Modified Raoult's Law; High-Pressure VLE; Henry's law; Chemical Reaction Equilibrium: Homogeneous and Heterogeneous reactions; Multi-reaction Equilibria; Liquid-Liquid Equilibria; Solid – Liquid Equilibria; Solid – Vapour Equilibria

Text Books:

1. J.M. Smith, H.C. Van Ness, M.M. Abbott, *Introduction to Chemical Engineering Thermodynamics*, 6th Ed., McGraw-Hill, 2001

2. S.I. Sandler, *Chemical, Biochemical and Engineering Thermodynamics*, 4th Ed., Wiley India, 2006

3. Y. V. C. Rao, *Chemical Engineering Thermodynamics*, 1st Ed., Universities Press, India, 1997

4. P. K. Nag, *Engineering Thermodynamics*, 5th Ed., Tata Mc-Graw Hill Education, 2013

Reference Books:

1. J.M. Prausnitz, R.N. Lichtenthaler, E.G. Azevedo, *Molecular Thermodynamics of Fluid-Phase Equilibria*, 3rd Ed., Prentice Hall, 1998

2. J.W. Tester, M. Modell, *Thermodynamics and its Applications*, 3rd Ed., Prentice Hall, 1999

3. R.C. Reid, J.M. Prausnitz, B.E.Poling, *Properties of Gases and Liquids*, 4th Ed., McGraw-Hill, 1987

CB208	Process Equipment Design-I	LTPC 1-0-3-5

Pre-Requisites: None.

Design Preliminaries, Design of cylindrical and spherical vessels under internal pressure, heads and closures, non-standard flanges, process vessels and pipes under external pressure, tall vessels, support for process vessels, thick walled high pressure vessels, shell and tube Heat Exchanger, Air Cooled Heat Exchanger, condensers and boilers, Material Specifications, Equipment fabrication and testing.

Text Books
1. B.C. Bhattacharya, *Introduction to Chemical Equipment Design, Mechanical Aspects*, 1st Ed., CBS publisher and Distributor, 1985

2. 2. M.V. Joshi, V.V. Mahajani, *Process Equipment Design*, 3rd Ed., Macmillan India Ltd., 1996

3. G. Towler, R. Sinnott, Butterworth-Heinemann, *Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design*, 4th Ed., An Imprint of Elsevier Inc., 2005

Reference Books:

1. M. S. Peters, K.D. Timmerhaus, R. E. West, *Plant Design and Economics for Chemical Engineers*, 5th Ed., McGraw Hill Education (India), 2003

2. J.R. Couper, W.R. Penny, J.R. Fair, S.M. Walas, *Chemical Process Equipment selection and design*, 3rd Ed., Elsevier Inc., 2012

3. R. H. Perry, D.W. Green, *Perry's Chemical Engineer's Handbook*, 7th Ed., McGraw Hill, 1998

Prerequisites: CB202 and CB203

List of Experiments Proposed:
1. **Mechanical Operations Lab:**
   a. Ball mill performance - MO1
   b. Plate and Frame Filter Press - MO2
   c. Cyclone Separator - MO3
   d. Jaw crusher performance - MO4
   e. Leaf Filter/Thickener - MO5
2. **Fluid Flow Lab:**
   a. Bernoulli's experiment - FF1
   b. Flow through pipe fittings - FF2
   c. Centrifugal Pump characteristics - FF3
   d. Venturi and Orifice meters - FF4
   e. Flow through packed beds - FF5

Standby:
1. Flow through Rectangular/V-notch - FF6
2. Pitot tube - FF7

Text Books:

1. W. L. McCabe, J. Smith and P. Harriot, *Unit Operations of Chemical Engineering*, 6th Ed., McGraw - Hill, International Edition, 2001

2. C. J. Geankoplis, *Transport Processes and Unit Operations*, 3rd Ed., Prentice Hall of India,1993

Prerequisite: Nil

Classification of chemical reactions; single, multiple, elementary and nonelementary homogeneous reactions; order and molecularity; temperature dependency; constant and variable volume batch reactor; reaction rate; rate constant; collection and interpretation of kinetic data; parallel and series reaction; batch, ideal plug flow and CSTR reactor design with and without recycle; temperature and pressure effects; Residence Time Distribution.

Text Books:

1. H. S. Fogler, *Elements of Chemical Reaction Engineering*, 2nd Ed., Prentice Hall, 1992

2. O. Levenspiel, *Chemical Reaction Engineering*, 3rd Ed., Wiley Eastern, 2003

Reference Books:

1. J. M. Smith, *Chemical Engineering Kinetics*, 3rd Ed., McGraw Hill, 1980

Prerequisites: CB204

Humidification/Dehumidification: Terminology and Definitions; Psychometric Chart; Cooling Towers.

Drying of Solids: Mechanism, Equilibrium, Drying Rate curve, Drying Calculations, Classification of Dryers, Dryer Selection and Design.

Crystallization: Solid-Liquid Phase Equilibrium, Nucleation and Crystal Growth, Crystal Size Distribution, Design of Crystallization Equipment.

Adsorption: Adsorbents – Characteristics and Properties, Adsorption Equilibrium - Isotherms, Adsorbent Selection, Adsorption Equipment, Pressure Swing Adsorption, Ion Exchange, Chromatography.

Membrane Separation: Membrane – Materials, Types, Preparation, Characterization and Modules, Reverse Osmosis, Dialysis, Micro Filtration, Ultra Filtration, Pervaporation.

Multi Component Distillation: Key Component, Approximate Method of design.

Text Books:

1. R. E. Treybal, *Mass Transfer Operations*, 3rd Ed., McGraw Hill, 1983
2. B. K. Dutta, Principles of Mass Transfer and Separation Processes, 8th Printing, PHI Learning Private Limited, 2015

Reference Books:

1. A. S. Foust, *Principles of Unit Operations*, 2nd Ed., Wiley, 1980

2. C.J. Geankoplis, *Transport Processes and Unit Operations*, 3rd Ed., Prentice Hall India, 1993

3. W. L. McCabe, J. C. Smith, P. Harriott, *Unit Operations of Chemical Engineering*, 7th Ed., McGraw Hill, 2005

Prerequisite: None.

Introduction and scope. Process Flow and Instrumentation Diagrams: Preparation, Symbols. Introduction to the following Industries including the Special Features of Design and Operation: Fuels and Industrial Gases including Natural Gas, Petrochemical and Downstream (in brief), Polymer, Fertilizer, Cement, Caustic Chlorine, Coal based Chemicals, Petroleum Refining Processes (in brief), Nitrogen and Its Derivatives, Sulphur and Its Derivatives, Phosphorus and Its Derivatives, Soaps and Detergents, Pulp and Paper, Alcohol based Chemicals, Specialty Chemicals.

Text Books:

1. J.A. Moulijn, M. Makkee, A.V Diepen, *Chemical Process Technology*, nd
2. C.E. Dryden, *Outlines of Chemical Technology*, Edited and revised by M. GopalaRao and Marshall Sitting, 2nd Ed., Affiliated East-West Press, 1973

   3. G.T. Austin, R.N. Shreve, *Chemical Process Industries*, 5th Ed., McGraw Hill, 1984

Reference Books:

1. P.H. Groggins, *Unit Processes in Organic Synthesis*, 5th Ed., McGraw Hill, 2001
2. D.F. Kirk-Othmer, *Encyclopedia of Chemical Technology*, 5th Ed.,
3. J.H. Gary, G.E. Handwerk, *Petroleum Refining: Technology and Economics*, 1st Ed., Marcel Dekker, 2001

4. S. Sarkar, *Fuels and Combustion*, 2nd Ed., Orient Longmans, 1990

Prerequisite: CB208

Basic Engineering design approach for pipe fittings and joints, reaction vessel and storage tank. Flowsheeting (includes Flowsheet Presentation, Process Simulation Programs, Flowsheets with Recycle, Flowsheet Optimization, Dynamic Simulation). Drawing and design of phase separation equipment such as hydro-cyclones, packed towers, plate columns, electro static precipitators. Design of Pressure relief system. Design of heat transfer equipment such as heat exchangers with and without phase change, evaporators, crystallizers. Design of mass transfer equipment such as distillation columns, absorption columns, extraction columns, dryers and cooling towers.

Text Books:

1. M. S. Peters, K.D. Timmerhaus, R. E. West, *Plant Design and Economics for Chemical Engineers*, 5th Ed., McGraw Hill Education, 2003
2. G. Towler, R. Sinnott, Butterworth-Heinemann, *Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design*, 4th Ed., An Imprint of Elsevier Inc., 2005
3. B. K. Dutta, *Principles of Mass Transfer and Separation Processes*, 8th Printing, PHI Learning Private Limited, 2015.

Reference Books:

1. J.R. Couper, W.R. Penny, J.R. Fair, S.M. Walas, *Chemical Process Equipment selection and design*, 3rd Ed., Elsevier Inc., 2012
2. R. H. Perry, D.W. Green, *Perry's Chemical Engineer's Handbook*, 7th Ed., McGraw Hill, 1998
3. B.C. Bhattacharya, *Introduction to Chemical Equipment Design, Mechanical Aspects*, 1st Ed., CBS publisher and Distributor, 1985
4. M.V. Joshi, V.V. Mahajani, *Process Equipment Design*, 3rd Ed., Macmillan India Ltd., 1996

CB309	Mass Transfer Lab	LTPC 0-0-3-3

Pre-Requisites: CB204

List of Experiments:

1. Measurement of Diffusivity of Carbon Tetrachloride in Air - MT1
2. Verification of Rayleigh's Equation for Batch Distillation - MT2
3. Separation of Two Miscible Liquids in a Sieve Plate Distillation Column - MT3
4. Loading and Flooding Characteristics during Counter-Current Flow through a Packed Column - MT4
5. Experiment on Continuous gas-solid adsorption of Carbon Dioxide onto Molecular Sieve - MT5
6. Performance Analysis of a Bench-Top Cooling Tower- MT6
7. Studies on Batch Drying and Generation of Drying Curve - MT7
8. Drying Characteristics of a Rotary Drier - MT8
9. Liquid-Liquid Extraction in a Packed Column - MT9
10. Batch Crystallizer - MT10
11. Generation of Vapour-Liquid Equilibrium Data - MT11
12. Separation of Two Miscible Liquids in a Bubble Cap Distillation Column - MT12

Text Books:

1. R. E. Treybal, *Mass Transfer Operations*, 3rd Ed., McGraw Hill, 1983
2. B. K. Dutta, *Principles of Mass Transfer and Separation Processes*, 8th Printing, PHI Learning Private Limited, 2015

Reference Books:

1. A. S. Foust, *Principles of Unit Operations*, 2nd Ed., Wiley, 1980
2. C.J. Geankoplis, *Transport Processes and Unit Operations*, 3rd Ed., Prentice Hall India, 1993
3. W. L. McCabe, J. C. Smith, P. Harriott, *Unit Operations of Chemical Engineering*, 7th Ed., McGraw Hill, 2005

Pre-Requisites: CB202 and CB203

List of Experiments:
Heat transfer lab
1. Thermal Conductivity of Metal - HT1
2. Finned Tube Heat Exchanger - HT2
3. Heat Transfer Through Composite Wall - HT3
4. Heat Transfer in Natural Convection - HT4
5. Shell and Tube Heat Exchanger – HT5
6. Drop-Wise and Film-Wise Condensation – HT6

Fuel Lab:
1. Proximate Analysis of Coal Sample – F1
2. Reid Vapour Pressure (RVP) of Gasoline – F2
3. Cloud Point and Pour Point of Heavy Oil – F3
4. Joule-Thomson Coefficient Apparatus– F4

Thermodynamics lab
1. Stefan-Boltzman Apparatus – HT7
2. Parallel and Counter-Current Heat Exchanger – HT8
3. Thermal Conductivity of Liquid – HT9
4. Calorific Value by Bomb Calorimeter – F5
5. Flash Point of Oil (Penske-Martens Apparatus) – F6
6. Partial Molar Enthalpies by Adiabatic Calorimetry – F7
7. Ebulliometric Determination of Vapour Pressures – F8

Text Books:

1. D. Q. Kern, *Process Heat Transfer*, 1st Ed., Mc-Graw Hill, 2001
2. J. P. Holman, *Heat Transfer*, 8th Ed., Mc-Graw Hill, 1996
3. G. G. Brown, *Unit Operations*, 1st Ed., CBS, 2005
4. S. Sarkar, Fuels and Combustion, 2nd Ed., Orient Longmans, 1990

Prerequisite: CB301

Review of Different Types of Reactors; Non-Ideal Flow Reactors; Concept of Residence Time Distribution (RTD), Segregation, Micro and Macro Mixing in Reactors, Methods of Obtaining RTD-E, F, C Curves, Mathematical and Experimental Techniques. Models of Non-Ideal Flow-Dispersion Models for the Case of Small or Large Extent of Dispersion.Effect of Dispersion on Conversion for General Irreversible Reaction Case.Tanks in Series Model-Effect of Number of Tanks on Conversion for General Irreversible Reaction Case. Recycle model. Multi parameter models. Diagnostic methods of analysis of flow patterns in reactors. Role of macro &micro-mixing& segregation in ideal (MFR, PFR) and non-ideal reaction cases.

Non-Catalytic Fluid Solid Reaction in Flow Reactors: (Excluding the portion covered under Reaction Kinetics) Applications to design of continuous solid flow reactors. Various design considerations. Application of fluid bed reactors and their design consideration. Heat transfer effects.

Solid Catalyzed Fluid Phase Reactor: Phenomena observed in operation of packed, fluid bed, slurry and such reactors. Product distribution in multiple and complex reactions. Thermal effects. Phenomenon of stability, unstability. Runaway and its analysis. Strategies for stable operations of reactors. Design considerations of fluid/solid catalytic reactors. Fluid bed reactors.

Design of Gas/Liquid and Liquid/Liquid and Gas/Liquid/SolidReactors: Heterogeneous reactors. Bubble heterogeneous reactors, Co-current & Counter-Current flow packed bed reactors.

Text Books:

1. H. S. Fogler, *Elements of Chemical Reaction Engineering*, Prentice Hall, 2nd Ed., 1992

2. O. Levenspiel, *Chemical Reaction Engineering*, 3rd Ed., Wiley Eastern, 2003

Reference Books:

1. J. M. Smith, *Chemical Engineering Kinetics*, 3rd Ed., McGraw Hill, 1980

CB304   Chemical Process Modelling and Simulation   LTPC 3-0-0-6

Prerequisite: CB201

Modeling: Fundamentals of mathematical models and formulation – Continuity equation, Equation of motion, Transport equations, Energy equation, Equations of state, Equilibrium, Chemical kinetics and their applications; Lumped and distributed parameter models – Fluid systems, CSTR (single, series, isothermal, constant hold up, variable hold up, gas phase pressurized and non-isothermal), Single component vaporizer, Multi-component flash drum, Batch reactor, Reactor with mass transfer, Ideal binary distillation column, Batch distillation, Heat exchanger, etc;

Simulation: Techniques of digital simulation – Information flow, from process to information flow diagram, From information flow diagram to numerical form, Recycles, Calculation of a recycle set, etc; Digital simulation of CSTRs in series, non-isothermal CSTR, Binary distillation column, Batch reactor, Computer aided design **Optimization:** Single variable optimization (analytical, dichotomous search, fibonacci, golden section, regulafalsi), Multivariable optimization (analytical, geometric programming, linear programming), Convergence methods (Newton's methods, direct substitution, Wegstein's method).

Text Books:

1. W. L. Luyben, *Process Modelling, Simulation and Control for Chemical Engineers*, 2 Sub Ed., McGraw Hill, 1989

2. S. S. Rao, *Engineering Optimization: Theory and practice*, 3rd Ed. New Age Publishers, 2013

3. A. K. Jana, *Chemical Process Modelling and Computer Simulation*, 2nd Ed., Phi Learning Pvt. Ltd., 2011

References Books:

1. B. V. Babu, *Process Plant Simulation*, Oxford University Press, 2004

2. A. Hussain, Gangaiah K., *Optimisation Techniques for Chemical Engineers*, Macmillan, 2001

3. B. W. Bequette, *Process Control: Modeling, Design and Simulation*, Prentice Hall India, 2006

4. K. Najim, *Process Modeling and Control in Chemical Engineering*, 1st Ed., CRC, 1989

Pre-Requisites: CB304

1. Steady state simulation of Heat Exchanger using ASPEN PLUS/ HYSYS;
2. Steady state simulation of a CSTR using ASPEN PLUS/ HYSYS;
3. Steady state simulation of Flash vessel using ASPEN PLUS/ HYSYS;
4. Steady state simulation of Distillation Column using ASPEN PLUS/ HYSYS;
5. Steady state simulation of an Absorption column using ASPEN PLUS/ HYSYS;
6. Dynamic simulation of Heat Exchanger using ASPEN PLUS/ HYSYS;
7. Dynamic simulation of a CSTR using ASPEN PLUS/ HYSYS;
8. Dynamic simulation of Flash vessel using ASPEN PLUS/ HYSYS;
9. Dynamic simulation of Distillation Column using ASPEN PLUS/ HYSYS;
10. Dynamic simulation of an Absorption column using ASPEN PLUS/ HYSYS

Text Books:

1. W. L. Luyben, *Process Modelling, Simulation and Control for Chemical Engineers*, 2 Sub Edition, McGraw Hill, 1989

Reference Books:

1. B. V. Babu, Process Plant Simulation, Oxford University Press, 2004
2. K. Najim, Process Modeling and Control in Chemical Engineering, 1st Ed., CRC, 1989

Prerequisite: MA 201

Principles of measurement, principles of transductions, Measurement of pressure, Temperature Level and flow measuring devices, composition measurements, selection of sensors, Electrical/Electronic/PLC control systems. Laplace Transform and Properties. Introduction to system dynamics, concept of dynamic response, linear systems, First, second and higher order system, systems with dead time. Definition of terms such as transfer function, time constant, gain of the process with practical examples. Response of the process to standard inputs. Introduction to process control: set point, disturbance, closed loop and open loop control, feedback and feed forward configurations, types of controllers including PI, PD and PID. Poles and zeros of the transfer functions. The effects of controller action on process response: offset, closed-loop gain, controller gain effect of controller parameters. Stability Analysis including Routh Test. Design of controllers using open loop response, Zigler-Nichols approach, experimental determination of process model. Introduction of frequency response technique: Design of controllers using frequency response technique, analysis of the systems for stability, Bode stability criterion. Multiple loop control systems, cascade control design, ratio control, feed forward control designs. Introduction to multivariable control system, Control strategies for common industrial processes such distillation, heat exchangers, etc. Control strategies for Batch processes.

Text Books:

1. D. R. Coughanowr, B. K. Lowell, *Process systems analysis and control*, 2nd Ed. McGraw-Hill, 1991

2. G. Stephanopoulos, *Chemical process control: An introduction to theory and practice*, PTR Prentice Hall Inc., 2008

Reference Books:

1.W. L. Luyben, Process Modelling, *Simulation and Control for Chemical Engineers*, 2 Sub Ed., McGraw Hill, 1989

CB310	**Chemical Reaction Engineering and Environmental Engineering Lab**	**LTPC 0-0-3-3**

Prerequisite: CB301

1. Study and operation of a packed bed reactor (CR-1);
2. Study and operation of a batch reactor(CR-2);
3. Study and operation of a CSTR(CR-3);
4. Study and operation of a plug flow reactor(CR-4);
5. Study and operation of a cascade CSTR(CR-5);
6. Study and operation of an adiabatic batch reactor(CR-5);
7. Study and operation Trickle bed reactor(CR-6);
8. Study and operation Condensation polymerization reactor(CR-7);
9. Study and operation Emulsion polymerization reactor(CR-8);
10. RTD study in a CSTR(CR-9);
11. RTD study in a plug flow reactor(CR-10);
12. Study and operation of a coiled tubular reactor(CR-11);
13. Determination of B.O.D and C.O.D (EE-1)

Text Books:

1. H. S. Fogler, *Elements of Chemical Reaction Engineering*, Prentice Hall, 2nd Ed., New Jersey, 1992

2. O. Levenspiel, *Chemical Reaction Engineering*, 3rd Ed., Wiley Eastern, 2003

Reference Books:

1. J. M. Smith, *Chemical Engineering Kinetics*, 3rd Ed., McGraw Hill, 1980

Prerequisite: MA201

Introduction. Vector and Tensor analysis. Molecular Transport Mechanisms.Newton's Law of Viscosity.Fourier's Law of Heat Conduction.Fick's Law of Diffusion. Transport in Laminar Flow or in Solids in One Dimension. Development of Continuity (conservation) Equations.Velocity, Temperature and Concentration Profiles.Equations of Change for Isothermal, Non-isothermal and Multi-component Systems.Equations of Motion for Free and Forced Convection (Heat / Mass). Momentum, Energy and Mass Transport in Boundary Layers with relevant analogies. Inter-phase / Unsteady State Momentum, Energy and Mass Transport.

Text Books:

1. R. B. Bird, W. E. Stewart, E. N. Lightfoot, *Transport Phenomena*, 2nd Ed., Wiley, 2006
2. F. P. Incropera, D. P. Dewitt, *Fundamentals of Heat and Mass Transfer*, 5th Ed., John Wiley & Sons Inc., 2010

Reference Books:

1. P. J. Pritchard, R. W. Fox, A. T. McDonald, *Introduction to Fluid Mechanics*, 8th Ed., John Wiley & Sons Inc., 2011
2. E. L. Cussler, *Diffusion: Mass Transfer in Fluid Systems*, 3rd Ed., Cambridge University Press, 2009

Prerequisite: CB308

List of Experiments Proposed:

1. Temperature Control Trainer – PC1
2. Pressure Control Trainer – PC2
3. Level Control Trainer – PC3
4. Flow Control Trainer – PC4
5. Characteristics of PLC Controller – PC5
6. Flapper Nozzle Assembly – PC6
7. Time Constant of Thermometer – PC7
8. Calibration of Thermocouple & Resistance Thermometer – PC8
9. Control Valve Characteristics – PC9
10. Pneumatic Controller – PC10

Standby:

1. Interacting & Non-interacting Systems – PC11
2. Multi Process Trainer – PC12

Text Books:

1. D. R. Coughanowr, B. K. Lowell, *Process systems analysis and control*, 2nd Ed., McGraw-Hill, 1991

2. G. Stephanopoulos, *Chemical process control: An introduction to theory and practice*, PTR Prentice Hall Inc., 2008

3. W. L. Luyben, *Process Modelling, Simulation and Control for Chemical Engineers*, 2 Sub Ed., McGraw Hill, 1989

Pre-Requisites: None.

Input information and batch versus continuous; input-output structure of the flow sheet; recycle structure of the flow-sheet; application of separation system principles for case studies; application of heat exchanger network design principles for case studies; cost diagrams and quick screening of process alternatives; preliminary process optimization; process retrofitting.

Equipment sizing and costing for different process units; Cost information, estimating capital and operating costs, total capital investment and total product costs, time value of money, measures of process profitability, simplifying economic analysis for conceptual designs, techno-economic feasibility report writing.

Text Books:

1. J. Douglas, *Conceptual Design of Chemical Processes*, McGraw Hill, 1989
2. M. S. Peters, K.D. Timmerhaus, R. E. West, *Plant Design and Economics for Chemical Engineers*, 5th Ed., McGraw Hill Education, 2003

Reference Books:

1. L.T. Biegler, I.E. Grossmann, A.W. Westerberg, *Systematic Methods of Chemical Process Design*, Prentice Hall, 1997
2. R. Smith, *Chemical Process Design*, McGraw Hill, 1995
3. E. E. Ludwig, *Applied Project Engineering*, 2nd Ed., Gulf Publishing Company, Houston, 1988

Departmental Electives

CB320	Catalysis Science and Engineering	LTPC 3-0-0-6

Introduction to catalysis; adsorption in solid catalysis; adsorption types and kinetics; multilayer adsorption and pore condensation

Heterogeneous catalysis: Synthesis methods (such as precipitation and co precipitation, sol gel method) and Characterization (using surface area analyzer, X- ray diffraction, FTIR, Raman, XPS, electron microscopy, thermal analysis); Catalyst test and reactor types; Reaction mechanism and rate equation; Kinetic analysis; External and Internal Transport; Catalyst deactivation; Steam Reforming and Petroleum Refining; Environmental Catalysis; Hydrogenation and oxidation catalysis

Homogeneous catalysis: Introduction and different types of reaction; Mechanism and kinetics; Industrial homogeneous process; Enzyme catalysis

Emerging catalysis: Zeolites catalysts; Polymerization catalysts; Carbon nanotubes; Nano metal or metal oxide catalysts; Phase transfer catalysts; Design of catalysis-supported and non-supported; Molecular Modeling

Text Books:

1. R. J. Farrauto, C. H. Bartholomew, *Fundamentals of Industrial Catalytic Processes*, Blackie Academic & Professional, 1997
2. H. S. Fogler, *Elements of Chemical reaction engineering*, Prentice – Hall of India, 2002
3. J.J. Carberry, *Chemical and catalytic reaction Engineering*, Dover Publications, 2001
4. J. M. Thomas, W. J. Thomas, *Principles and Practice of Heterogeneous Catalysis*, VCH, 1997

References Books:

1. J. M. Smith, *Chemical Engineering Kinetics*, McGraw-Hill Book Company, 1981
2. D.M. Ruthven, *Principle of adsorption & adsorption processes*, John Wiley & sons, 1984
3. C. H. Bartholomew, R. J. Farrauto, *Fundamentals of Industrial catalytic Processes*, Wiley- VCH, 1997
4. B. Viswanathan, S. Sivasanker, A.V. Ramaswamy, *Catalysis: Principles & Applications*, CRC Press, 2002

CB322	Energy Management	LTPC 3-0-0-6

Importance of energy management. Energy audit: method, analysis of plant data, energy balance, laws of thermodynamics, measurements, portable and on line instruments. Utility Systems: Boiler -efficiency testing, excess air control, Steam distribution & use- steam traps, condensate recovery, flash steam utilization. Thermal insulation. Electrical systems: Demand control, power factor correction, load scheduling/shifting, Motor drives-efficiency testing, energy efficient motors, motor speed control. Lighting- lighting levels, efficient options, day lighting, timers, Energy efficient windows. Energy conservation in pumps, Fans (flow control), Compressed Air Systems, Refrigeration & air conditioning systems. Waste heat recovery: heat pipes, heat pumps. Cogeneration - concept, options (steam/gas turbines/diesel engine based), selection criteria, control strategy. Heat exchanger networking- concept of pinch, target setting, problem table approach, composite curves. Demand side management. Production planning and management.

Text Books:

1. L.C.Witte, P.S.Schmidt, D.R.Brown, *Industrial Energy Management and Utilization*, Hemisphere Publ, Washington,1988

2. I.G.C.Dryden, *The Efficient Use of Energy*, Butterworths, London, 1982

3. W.C.Turner, *Energy Management Handbook*, Wiley, New York, 1982

Reference Books:

1. Technology Menu for Efficient energy use- Motor drive systems, Prepared by National Productivity Council and Center for & Environmental Studies- Princeton Univ., 1993.
2. Industrial Energy Conservation Manuals, MIT Press, Mass, 1982

Introduction to Bioprocesses: Traditional and modern bioprocess Engineering-overview, integrated bioprocess, upstream and downstream operations, process flow sheets; Material balance and Energy balance for different systems; Stoichiometry of cell growth and product formation; Energetic analysis of microbial growth and product formation; thermodynamic efficiency of growth, Enzyme technology- Enzyme kinetics, immobilization and industrial production. Fermentation Processes: Fermentation processes-outline, overview & types, design, parameteres& construction of fermentor and ancillaries; application in the biotechnology industry; kinetic models for microbial growth; behavior of microbes in different reactors; Media design: requirements for fermentation processes and optimization techniques (placket Burman Design). Separation technology: Solids removal operations - settling, centrifugation and filtration; Product isolation - adsorption and extraction; Purification techniques - precipitation, ultrafiltration, chromatography and electrophoresis; Product polishing operations-crystallization and drying; Integrated bio-reaction and bio-separation processes-membrane bioreactors, extractive fermentation. Bioprocess Engineering and Industry:

Environmental biotechnology - wastewater engineering, bioremediation; Bioprocess instrumentation; Biological systems for the production of commercial goods and services: foods, feed, pharmaceuticals, nutraceuticals, chemicals, polymers, fuels, equipment, diagnostics and other biomaterials; good manufacturing practices, Safety and regulatory issues.

Text Books:

1. Michael L. Shuler, Fikret Kargi, *Bioprocess Engineering Basic Concepts*, 2nd Ed., Prentice Hall PTR, 2014

4.　　**Reference**

1.Pauline M. Doran, *Bioprocess Engineering Principles*, 2nd Ed., Academic Press,

Introduction: History of fuels, Types and properties of Fuels

Solid Fossil Fuel (Coal): Coal classification, composition, basis; coal mining; Combustion of coal and coke making; coal liquefaction; coal gasification; clean coal technology Liquid Fossil Fuel (Petroleum): Exploration and evaluation of crude petroleum; Distillation; Cracking; Coking; Reforming of naphtha; Hydrotreatment, dewaxing, deasphalting

Gaseous Fuels: Natural gas and LPG; Producer gas; Water gas; Hydrogen; Acetylene; Other fuel gases

Combustion Technology: Fundamentals of thermochemistry; Combustion air calculation; Calculation of calorific value of fuels; Adiabatic flame temperature calculation; Mechanism and kinetics of combustion; Flame properties; Combustion burners; Combustion furnaces; Internal combustion engines

Text Books:

1. *Modern Petroleum Technology*, Vol 1, Upstream, Ed. by Richard A. Dave, IP, 6th ed., John Wiley & Sons. Ltd.
2. *Modern Petroleum Technology*, Vol 2, Downstream, Ed. by Alan G. Lucas, IP, 6th ed., John Wiley & Sons. Ltd.
3. Irvin Glassman, Combustion, 2nd Ed., Academic Press.
4. 4. B.K. BhaskarRao, Modern Petroleum Refining Processes, 4th Ed., Oxford & IBH Publishing Co. Pvt. Ltd.

Reference Books:

1. Report on the project "Coal Combustion Study", sponsored by Tata Tron and Steel Company Ltd., Jamshedpur
2. John Griswold, *Fuels Combustion and Furnaces*, Mc-Graw Hill Book Company Inc.
3. Samir Sarkar, *Fuels and Combustion*, 3rd Ed. Universities Press.
4. W.L. Nelson, *Petroleum Refinery Engineering*, 4th Ed. Mc-Graw Hill Book Company

CB424   Numerical Methods in Chemical Engineering   LTPC 3-0-0-6

Solution of simultaneous linear and non-linear equations; Eigenvalues and eigenvectors of matrices; Statistical analysis of data; Curve fitting; Approximation of functions; Interpolation; Numerical integration and differentiation; Solution of ordinary differential equations - initial and boundary value problems; Solution of partial differential equations; Analysis of error and stability in numerical computing; Implementation of numerical methods on computer through programming in FORTRAN/C++ and commercial software such as MATLAB, NAG and IMSL routines.

Text Books:

1. S. C. Chapra, R. P. Canale, *Numerical methods for engineers*, 7th Ed. Tata-McGraw-Hill, 2015
2. S. K. Gupta, *Numerical methods for engineers*, New Age International, 2001

Reference Books:

1. A. Constantinides, *Applied numerical methods with personal computers*, McGraw-Hill, 1987
2. F. Gerald, P. O. Wheatley, *Applied numerical methods*, Pearson Education, 2003
3. R. M. Somasundaram, R. M. Chandrasekaran, *Numerical methods with C++ programming*, Prentice-Hall of India, 2005
4. W. H. Press, S. A. Teukolsky, W. T. Vellerling, B. P. Flannery, *Numerical recipes inFORTRAN: the art of scientific programming*, Cambridge University Press, 1992

CB426   Petroleum Refinery and Petrochemicals   LTPC 3-0-0-6

Origin and occurrence, composition, classification and physico-chemical properties of petroleum; testing and uses of petroleum products; refining Processes such as distillation, cracking, reforming; conversion of petroleum gases into motor fuel, aviation fuel; lubricating oils and petroleum waxes; chemicals and clay treatment of petroleum products, desulfurization; refining operations -Dehydration, Desalting, Gas separation, Natural gas production and gas sweetening; tube still heater design; product profile of petrochemicals; petrochemical feed stocks; olefin and aromatic hydrocarbons production; Treatment and upgrading of olefinic C4 and C5 cuts; chemicals from C1 compounds, ethylene and its derivatives, propylene and its derivatives, butadiene and butene; BTX chemicals.

Text Books:

1. W.L. Nelson, *Petroleum Refinery Engineering*, McGraw Hill, New York, 1961
2. K. H. Altgelt, M. M. Boduszynski, *Composition and analysis of heavy petroleum fractions*, Dekker,1994

Reference Books:

1. J. H. Gary and G. E. Handwork, *Petroleum refining technology and economics*, 4th Ed., Dekker, 2001

Biofuels: Classification – Biomass production for energy forming – Energy through fermentation – Pyrolysis – Gasification and combustion - Biogas - Aerobic and Anaerobic bio conversion process - Feed stock - Properties of bio-gas composition - Biogas plant design and operation.

Hydrogen Energy: Electrolytic and thermo chemical hydrogen production – Metal hydrides and storage of hydrogen – Hydrogen energy conversion systems hybrid systems
– Economics and technical feasibility.

Solar Energy: Solar radiation - availability- Measurement and estimation- Isotropic and anisotropic models- Introduction to solar collectors (liquid flat- Plate collector - Air heater and concentrating collector) and thermal storage- Steady state transient analysis- Photovoltaic solar cell - Hybrid systems - thermal storage- Solar array and their characteristics evaluation – Solar distillation – Solar drying.

Ocean Thermal Energy Conversion: Geothermal - Wave and Tidal energy - Availability - Geographical distribution - Power generation using OTEC - Wave and Tidal energy - Scope and economics - Geothermal energy - Availability - Limitations.

Wind Energy: Wind energy - General considerations - Wind Power plant design – Horizontal axis/Vertical axis wind turbines - Design considerations - Number of blades - Blade profile - Power regulation - Choice of power plant - Wind mapping and selection of location-Cost analysis and economics of the systems.

Text Books:

1. D. Merick, R. Marshall, *Energy, Present and Future Options*, Vol. I and II, John Wiley and Sons, 2001
2. M. V. R. Koteswara Rao, *Energy Resources-Conventional and Non-Conventional*, 2nd Ed., BS Publications, 2006
3. B.H. Khan, *Non-Conventional Energy Resources*, 2nd Ed., Tata McGraw Hill, 2009
4. C. S. Solanki, *Renewable Energy Technologies: A Practical Guide for Beginners*, Second Printing, PHI Learning Private Limited, 2009

Reference Books:

1. G.W. Koeppl, *Patnam's power from wind*, Van Nostrand Reinhold Co., 2002
2. J.D. Ritchie, *Source Book for Farm Energy Alternative*, McGraw Hill, 1999
3. J.W. Twidell, A.D. Weir, *Renewable Energy Resources*, ELBS, 1999
4. D. Mukherjee, S. Chakrabarti, *Fundamentals of Renewable Energy Systems*, New Age International (P) Limited, 2005

CB501	**Molecular Modeling and Simulation**	**LTPC 3-0-0-6**

Pre-requisite: Not required   **Total Lectures (42)**

I. Introduction (1)

Popular models for chemical and biological systems with examples.

II. Statistical Thermodynamics (6+2)

Micro canonical ensemble and the ergodic hypothesis; Canonical ensemble and Boltzmann probability; Thermodynamics and the Boltzmann equation for entropy; Isobaric and grand-canonical ensembles; Partition function for different ensemble; Exercise-1: (Calculating Macroscopic Properties from molecular level)

III. Models and Force fields (2+1)

Model hierarchy; Force field in molecular modeling; Short-range forces: cutoff, correction; Electrostatic forces: Ewald summation; reaction field; Construction of force field; External force;
Exercise-2: (Calculation of long range correction using different methods)

IV. Molecular dynamics (6+4)

Newton equations of motion; Verlet method; Leap-frog method; Velocity Verlet; Thermostats: based on the Maxwell-Boltzmann distribution, based on velocity rescaling (Berendsen method), Nosé-Hoover method (qualitatively); Equilibrium and non-equilibrium molecular dynamics
Exercise-3: Comparison of various thermostats.
Exercise-4: Molecular Dynamics for simple LJ system

V. Monte Carlo methods (4+2)

Metropolis method; Markov chains; Acceptance ratio; Different moves: translation, rotation, volume change;
Exercise-5: Monte Carlo Simulation for simple LJ system

VI. Simulation methodology (4+2)

Equilibration and Production Cycle, Boundary conditions; Mechanical quantities: temperature, internal energy, pressure; Entropic quantities (thermodynamic integration, Widom, local density method)

Exercise-6: Molecular dynamic simulation for simple LJ system.

VII. Structural and Kinetic Properties   (2+2)

      Radial distribution function; Structure factor; Diffusion, Viscosity
Exercise-7: RDF, Diffusion and Viscosity of Simple LJ system

VIII. Simulation for Molecular systems   (2+2)

      Polar Molecules like water; Chain Molecules like surfactants; Cyclic
compounds; Polymers; Protein etc
      Exercise-8: Simulation for complex molecules.

Text Books:

    1. D. Frankel, B. Smit, *Understanding Molecular Simulation: From algorithm to Applications*, 2nd Ed., Elsevier, 2002

    2. M.P. Allen, D. J. Tildesley, *Computer Simulation of Liquids (Reprint/Revised)*, Clarendon Press, 1989

    3. Donald McQuarrie, *Statistical Thermodynamics (Reprint/Revised)*, University Science Books, 1991

Reference Books:

    1. D.C. Rapaport, *The Art of Molecular Dynamics Simulation*, 2nd Ed., 2004
    2. D. Chandler*, Introduction to Modern Statistical Mechanics*, OUP USA, 1987

| **CB503** | **Process Integration** | **LTPC 3-0-0-6** |

Process Integration; Targeting for energy, Area, unit and cost; Heat exchanger network design and evolution: Heat exchanger design, Retrofit design; Mathematical optimization techniques; Process integration of different systems: fired heater, Cogeneration and utility system, Solar thermal, Batch Process, distillation column, evaporators, Resource management: Water management, Hydrogen management, Environmental management; Recent developments.

Text Books:

1. I.C. Kemp, *Pinch Analysis and Process Integration-A User Guide on Process Integration for the Efficient Use of Energy*, Elsevier, 2007

2. U. V. Shenoy, *Heat Exchanger Network Synthesis: Processes Optimization by Energy and Resource Analysis*, Gulf Publishing Company, Houston, 1995

Reference Books:

1. B.D. Linnhoff, W. Townsend, D. Boland, G. F. Hewitt, B. E. A. Thomas, A. R. Guy, R. H. Marsland, *User Guide on Process Integration for the Efficient Use of Energy*, The Institution of Chemical Engineers, Rugby, UK, 1982

2. J. M. Douglas, *Conceptual Design of Chemical Processes*, McGraw-Hill, New York, 1988