Syllabi of courses required for the 4 Semester
M. Tech. Examination in Chemical Engineering
University of Calcutta

Semester I
Theoretical Papers

Abel’s equation – analysis of solution: separable and non separable Kernels: iterative methods of solution.
Introduction to some new mathematical tools – fuzzy set, G. A.

Paper – II (MChE–102): Core – II: Transport Phenomena [3 – 1 – 0] [4 Cr]
Vectorial treatment of transport processes.
Stability of flows
Detailed treatment of boundary layer and turbulent flows with heat and mass transfer.
Analogies of turbulent transport.
Multicomponent diffusion, Macroscopic balances for Multicomponent systems. Interphase Transport in Multicomponent systems.
Mass transfer with chemical reaction. Mass Transfer with high flux.
Simultaneous heat and mass transfer
Analysis of heat and mass transfer with phase change.
Non-Newtonian fluid mechanics; Heat and Mass transfer in non-Newtonian flows.

Modeling of systems: heat exchangers, reactors, distillation columns, etc.: steady state and dynamic models – deterministic and stochastic systems.
Simulation of process systems.
**Specialization - Process Engineering: Process Engineering I**
Scope of process engineering and the role of a process engineer.  
Process and technology selection, discrimination between available alternatives.  
Engineering flow diagrams: logistics of flow sheets and flow diagrams – types of drawing issues, internal communication archives.  
Process piping systems: materials selection, piping calculations, sizing for single and multiphase flow.  
Process vessels: design criteria, selection specifications.  
Review of pumps, fans, blowers, compressors: performance characteristics, selection and specification.  
Mixing and agitation systems: Thermal insulation. Process synthesis and Flowsheeting.

**Specialization - Petrochemicals and Petroleum Refining, Engineering: Petroleum Science**
Crude composition – elemental, chemical nature of components, category of components – PONA etc. Oil, resin, asphaltene etc., structure of components.  
Physicochemical properties of crude and hydrocarbons.  
Density, Surface tension, Critical properties, Viscosity, Electrical conductivity, acent factor, Freezing point, Thermal conductivity, Compressibility, Boiling point, Diffusivity, Vapour pressure, Specific Heat, enthalpy, entropy etc. correlation-connecting the properties to one another, to molecular weight and structure.  
Physical properties. Crude, Petroleum fluids, density, boiling point refractive index surface tension correlative parameters – API, UOPK, CI (Correlative Index), Viscosity Gravity Index, Compressibility, Thermal expansion Important Specification parameters – Aniline point, Smoke point, RVP, relationship between properties and chemical nature and different property correlations for crude and other petroleum fluids.  
Thermodynamics: P-V-T properties of petroleum fluids (gases and liquids); Phase equilibria, Critical region and supercritical phenomena, hydrates Solubilities of solids, liquids and gases, Tuning of equation of state.  
Reservoir fluid types - Black oil to dry gas, Petroleum rheology / flow properties  
Chemical reaction – Chemistry of hydrocarbons – reaction – oxidation – slow, catalytic, combustion, explosion, Cracking – thermal and catalytic, hydrogenation, dehydrogenation, polymerization, isomerization.  
Basic reaction thermodynamic data – compound stability, mechanism of reactions, and Rates of reaction – reaction rate theories, models and methods and other related basic chemistry/statistical /quantum mechanics, reactions in solutions.  
Catalysts and Catalytic process - Acid catalysed reactions - Acidity function, different acids, super acids.  
Types of reactions catalysed by acids, mechanisms, rates models; Zeolites – structures and properties.  
Types, Catalytic effects, shape selectivity, size selectivity Active sites, Poisoning of Catalysts; Hydrogenation/dehydrogenation catalysts.  
Other reaction involving hydrocarbons - Halogenation, alkylation, production reactions, Aromatic hydrocarbon reaction  
Chemistry of associated compounds - Non hydrocarbons present in crude, entering as common impurities/produced during processing or added/used for processing – chemical/physical properties, reactions, solubilities, phase equalibrium, property correlations.
Specialization – Environmental Engineering: Industrial Hazards and Plant Safety
Engineering ethics, Nature of accident in processes, Major chemical plant accidents in India and abroad, Applicable safety norms, rules and regulation. Fundamentals of toxicology, toxic effects of pollutants on the ecosystem, Dose-response relationships, Threshold limit values, government regulations.
Material safety data sheets (MSDS), Monitoring techniques for evaluation of worker exposure to toxics vapours, dust and noise, control technologies, respirators, ventilation.
Source models for accidental release of pollutants from a chemical plant, estimation of flow of liquids and vapours from a leak, hole, pipe etc., adiabatic and isothermal flows, flashing liquids. Detailed study on the derivation and application of Pasquill –Gifford and other dispersion models. Fire triangle and explosion, flammability characteristics of liquids and vapours, dependence on temperature and pressure, autoignition, autooxidation, adiabatic compression, spray and mists. Detonation and deflagration, confirmed explosion, vapour cloud explosions, BLEVE, Blast and missile damage, energy of mechanical and chemical explosions. Corrective control technologies to prevent fire and explosions, vacuum and pressure purging, sweep-through and diaphragm purging. Fundamentals of static charge development, accident potential and control techniques.
Explosions proof instruments, ventilation and sprinkler system. Relief system, sizing relief valves, deflagration venting for dust and vapour, rupture discs, flanges, scrubbers and condensers. HAZOP and HAZAN, fire and Explosion index, event and fault trees, probability of coincidence and failures, safety reviews. Case studies.

Specialization – Biotechnology: Biotechnology Fundamentals

Specialization - Process Engineering: Process Engineering II
Specialization - Petrochemicals and Petroleum Refinery Engineering: Petroleum Geology, Petroleum Economy, Safety and Environment

Elementary ideas on petroleum geology.
Reservoir engineering; Fundamental concepts – Flow characteristics of reservoirs, Reservoir drilling mechanisms, Basic equations and tools. Pressure maintenance, Improving oil recovery;
Waste generation in petroleum oil refineries and petrochemical plants;
Waste water treatment in reference to Petroleum Oil Refining Operations and Petrochemical Plants (including spent caustic treatment, and other treatment suggested in Indian Regulations)
Air emission control in reference to particulate collection (for instance in FCCU), gas cleaning (e.g., \( \text{H}_2\text{S}/\text{CO}_2; \text{SO}_2 \)); NOx control methodologies; Claus / Super Claus Sulfur Recovery Process; VOC control – its need and related technologies.
Hazardous waste management in petroleum oil refineries and petrochemical plants.

Paper – V (MChE–153): Elective II

Specialization - Environmental Engineering: Water Pollution and Waste Water Treatment

Sampling of waste water; Analytical and instrumental techniques for measuring various parameters specified in the effluent discharge standards.
Waste Water Treatment Methodologies: Pre-treatment, Primary Treatment, Secondary Treatment, Tertiary Treatment;
Physico-Chemical Treatment: Screening, Grit Chambers, Equalization, Sedimentation/Clarification, Flocculation, Floatation, Aeration, Granular Media Filtration, Chemical Precipitation, Disinfection.
Biological Treatment: Fundamentals of microbiology; Kinetics of biological growth, Aerobic/Anaerobic and Suspended/Attached growth processes; Design of aerobic processes (Activated Sludge Process; Trickling Filter, Oxidation Ditch, Rotating Disc Contactor; Stabilization Ponds; Aerated Lagoons); Design of anaerobic processes (UASB, Filters, Fluidized/Expanded Bed Systems).
Paper – V (MChE–154): Elective II

Specialization – Biotechnology: Molecular Biology and Genetic Engineering

Practical Papers

Solving problems using computational techniques. Programs to be written through C- language. Familiarization of MATLAB.

The candidate shall have to select a suitable topic and to prepare a comprehensive report on it. The candidate shall have to make an oral presentation of the report prepared, in a seminar. The report should be submitted at the time of the seminar.
Semester II
Theoretical papers

Paper – I (MChE–201): Core – IV  
[3 –1 – 0] [4 Cr]

Paper – II (MChE–202): Core – V  
[3 –1 – 0] [4 Cr]

Core – IV and Core – V:
Department will offer courses in such a way so that students will take two courses from the following five papers as Core – IV and Core – V

(a) Reaction Engineering
Theories of reaction rates – homogeneous, heterogeneous and catalytic process.
Kinetics of complex reactions.
Catalysis: Heterogeneous catalytic reactions; Model discrimination and parameter estimation; Inter-phase and intra-phase transport effects.
Non-catalytic gas-solid reactions – transport models.
Gas-liquid reactions.
Special reactions: Polymerization, fermentation, photochemical and electrode reactions.
Non-ideal flow patterns, population balance, transport models.
Multiphase reactor design.
Stability of reactors: Lumped and distributed parameter systems; Stability of multiphase reactors.

(b) Statistical Thermodynamics
A few concepts from quantum mechanics: Introduction, The Schrodinger wave equation, Particle in a box.
The statistical bases of thermodynamics: Microscopic and macroscopic thermodynamics, Contact between statistics and thermodynamics, the classical ideal gas, Entropy of mixing and the Gibbs paradox.
Fluctuations and equivalence of ensembles: Fluctuations: energy of a closed system; open isothermal system; in volume in an isothermal, isobaric system. Thermodynamic equivalence of ensembles: system partition function and particle partition function.
Deductions of partition functions and their application to evaluate macro-thermodynamics of ideal gases: monoatomic molecules, diatomic molecules, polyatomic molecules.
Deduction of $g^B$, Excess Gibbs energy expression for a binary mixture from the Lattice Theory using canonical partition function (CPF), Evaluation of excess entropy of a polymer solution, High pressure vapor liquid equilibria from generalized van der Waals partition function.
Principle of equipartition of energy.
Chemical reaction equilibrium: Equilibrium constant – Statistical approach, Isomerization reaction, Isotopic exchange reaction equilibrium, Dissociation of diatomic molecules, A general chemical reaction, Statistical mechanics of interacting system: The method of cluster expansion:– Cluster expansion for a classical gas, Virial expansion of the equation of state, Evaluation of the virial coefficients.
Phase transitions: Criticality, Universality and scaling:– Problem of condensation, Condensation of a van der Waals gas, Dynamic model of phase transition, The lattice gas and the binary alloy, Isuing models zeroth / first approximation, Mean field theory, Connecting van der Waals EOS model to statistical mechanics, Hard sphere fluid, Perturbed hard sphere fluid.
Foundation of molecular simulations, Monte Carlo and molecular dynamics.
Application of molecular simulation to estimate pure component and mixing properties.

(c) **Process Dynamics and Control**
Multiple input – output system, non-linear processes.
Advanced controls-feed forward, cascade, ratio, adaptive, split range, artificial neural net, fuzzy logic.
Analog versus digital system – direct digital, indirect digital controls, supervisory control, DCS.
Computer controlled system- hardware and software
Sampled data system- Z transform, pulse transfer functions, feedback loop response analysis, stability analysis
Process identification, model predicted control adaptive control
Robust control analysis- in SISO, MIMO system
Dynamic simulation and control techniques

(d) **Product Design**
Basic ideas of process synthesis. Network (Heat Exchanger and Mass Exchanger) analyses.
Correlating property change with structure and physical treatment.
Structural or other changes needed for obtaining polymers with modified property – basic concept, examples with descriptions.
Membrane sensitization with ions and chemicals.
Changes in recent demands of specialty product.
Relationship among composition, chemical structure, physical treatment with material properties.
Synthesis of production routes, concepts of specific catalyst, self organizing structure.

(e) **Optimization Methods in Chemical Engineering**
Introductory concepts : Objective function. Stationery point.
Relative and Absolute extrema. Convex and Concave functions.
Optimization of functions of one or more variables: Analytical techniques for unconstrained optimization necessary and sufficient conditions for an extremum.
Numerical technique with constrained optimization.
Linear programming : Properties of convex sets.
Non-linear programming, penalty function technique.
Geometric programming.
Integral programming.
Dynamic programming, Dynamic systems, Principles of optimality, Multistage optimization, Discrete and Continuous Dynamic programming
Numerical search techniques, Direct search, Gradient method, Quadratic Convergence technique
Variational methods: basic principles, the continuous maximum principle, Hamiltonian function and application.trajectory optimization.
Applications of the above techniques to chemical engineering systems.
Paper – III (MChE–231): Elective III

Specialization - Process Engineering: Process Synthesis
Synthesis of separation trains: the task of separation: importance of distillation column sequencing: heuristic rules; procedure of optimal sequencing.
Reliability consideration and hazard analysis.


Specialization - Petrochemicals and Petroleum Refinery Engineering: Refinery Engineering


Specialization - Environmental Engineering: Air Pollution and Control
Nature and composition of the atmosphere; Fundamentals of atmospheric chemistry; Carbon, sulfur and nitrogen cycles; Air pollutants and their toxicity. Applicable Acts, Rules and Regulations for the prevention and control of air pollution; Air emission standards for Process Industries; Sources and typical characteristics of industrial air pollution emphasizing categorization of Industries under Indian Regulations.
Air Quality Monitoring; Stack gas monitoring; Analytical and instrumental techniques for measuring various parameters specified in the Air Emission Standards.
Atmospheric dispersion of pollutants; Application of dispersion modeling in stack design.
Special emphasis will be given for operation of hybrid gas cleaning devices, Flue Gas Desulfurization, NOx control processes, Bioscrubbers / Biofileters; CO2 Capture processes.
Fundamentals of noise pollution; Hearing damage and other health effects, Standards of noise in various work places; Monitoring of noise level; Noise control techniques.

Paper – III (MChE–234): Elective III

Specialization – Biotechnology: Biochemical Engineering
Microbial growth kinetics, aerobic and anaerobic growth transition. Growth and nongrowth associated product formation.
Batch and continuous fermentation. Conventional and nonconventional bioreactors.
Enzyme reactor system. steady state analysis of mass transfer and biochemical reactions in enzyme catalysed reactors. transient analysis of immobilized enzyme reactions.

Rheology of fermentation broth. transport phenomena in bioprocess. bioreactor design and scale up. imperfectly mixed bioreactor system. instrumentation and control of bioreactors.

Paper – IV (MChE–241): Elective IV [3 – 1 – 0] [4 Cr]

Specialization - Process Engineering: Industrial Engineering
Industrial Engineering Principles – Historical development, introduction to work study, the human factor. Network Analysis in Project Planning – Network diagram, Analysis of project through Network diagram, Upgrading of network, Financial planning through network, Network crashing, Allocation of Resources in project, Programme evaluation and review technique (PERT) Operations research – What is operations research, Historical development of operations research, methodology of operations research, operations research techniques, operations research models. Application of linear programming techniques in real life situations, Sensitivity Analysis. Inventory control – Terminologies connected with Inventory control, Basic Inventory control models, Economic order quantity, Extension of EOQ model, Analysis of Lead time, Periodic review model, optimal replenishment inventory system

Waiting line problem – Characteristic of queueing system, Notations and symbols, Queueing system as a stochastic process, The M/M/I system, The M/M/C system


Paper – IV (MChE–242): Elective IV [3 – 1 – 0] [4 Cr]

Specialization - Petrochemicals and Petroleum Refinery Engineering: Petrochemicals
Major petrochemicals: synthesis gas, C_1, C_2, C_3, C_4 hydrocarbons and aromatics – their derivatives, major competitive processes – alternative routes, commercial production, process and plant descriptions, design and safety aspects.

Monomers for the synthesis of elastomers.
Monomers for polyamide synthesis.
Monomers for polyester synthesis.
Monomers for polyurethane synthesis.

Fundamentals of polymer chemistry, Commercial production of different polymers – process and plant description, design and safety aspects.

Paper – IV (MChE–243): Elective IV [3 – 1 – 0] [4 Cr]

Specialization - Environmental Engineering: Solid Waste Management and Environmental Management Systems

Municipal Solid Waste Management (MSW): Types, Sources and Pollution Potential of MSW; Rules and Regulations for MSW Management. MSW Management: Generation, on-site storage, collection, separation, processing and disposal (sanitary landfill, biological digestion etc.).

Bio-Medical Waste Management: Introduction to BMW; Types, Sources and Pollution Potential of BMW; Rules and Regulations for BMW Management. BMW Management: Generation, on-site storage, collection, transportation, separation, processing and treatment / disposal.

Hazardous Waste (HW) Management: Introduction to HW; Definition of HW; Types, Sources and Pollution Potential of HW; Rules and Regulations for HW Management. Characterization and site assessment, Transport models for entry of hazardous pollutants from soil into groundwater. HW Treatment and Disposal: Air/Steam venting; Bio Remediation; Chemical Treatment; Fixation and Stabilization; Engineered Land Filling; TSDF for Hazardous Wastes.

e-Waste Management: Introduction to e-Waste, Sources and Pollution Potential of e-Waste; Rules and Regulations for e-Waste Management. Definition, classification & component analyses of e-Waste; e-
Waste Management: Generation, on-site storage, collection, transportation, separation, processing and treatment / disposal. Integrated Solid Waste Management Practices.

*Environmental Management Systems:* Environmental management: problems and strategies; Sustainable Development; Transboundary movement of prohibitive wastes. Definition and measurement of environmental impact; Environmental Impact Assessment (EIA), EIA methodologies; EIA Notification in India, ISO:14000 series of international environmental management systems; Environmental Auditing; Life Cycle Analysis.

**Paper – IV (MChE–244): Elective IV**

**Specialization – Biotechnology: Bioprocess Modeling and Simulation**

- Characteristics of biological system and process. Modeling of simple systems.
- Monod Chemostal Model and effect of recycle.
- Non-ideal flow bioreactors.
- Modeling of conventional and nonconventional bioreactors like CSTR, PFTR, Fluid bed, Film reactor etc.
- Modeling of biological waste treatment processes.
- Steady and dynamic simulation of fermentation process.
- Simulation of some biological systems and processes.

**Practical Papers**


- Study of flow sheeting problems. Writing and uses of dynamic simulation programmes. Students require to submit two copies of type-written report on the assigned problem.

**Paper – V (MChE–252): Laboratory**

**Specialization - Petrochemicals and Petroleum Refinery Engineering: Petroleum Laboratory**

- Standard testing methods for crude and distillation e.g. A.S.T.M and TBP distillation. Sulfur determination.
- Carbon residue smoke point flash point aniline point pour point cloud point viscosity, viscosity index, reid vapour pressure, drop point of grease.
- Catalytic and non-catalytic reaction studies; Azeotropic and extractive distillation
- Liquid-liquid equilibrium and extraction
- Light end analysis, PONA analysis by chromatography and instrumental methods

**Paper – V (MChE–253): Laboratory**

**Specialization - Environmental Engineering: Environmental Engineering Laboratory**

- Water and Waste Water Analysis: pH, Dissolved Oxygen, BOD, COD, Total Suspended Solids, Total Dissolved Solids, TOC, Turbidity, Electrical Conductivity, Oil & Grease, Heavy Metals, Fluoride, Phenolics, Cyanide, other characteristic compounds listed in Indian standards.
- Ambient Air Quality Monitoring: Monitoring of PM$_{2.5}$, SPM, SO$_2$, NO$_x$ using High Volume Sampler.
- Stack Gas Monitoring: Determination of Stack Gas Velocity by Pitot Tube; Determination of moisture content and CO$_2$ in the flue gas; Stack gas monitoring under iso-kinetic conditions.

**Paper – V (MChE–254): Laboratory**

**Specialization – Biotechnology: Biotechnology Laboratory**

2. Preparation of nutrient broth media. Techniques of pure culture, isolation and identification of microbes
3. Extraction of DNA and estimation. RNA extraction and estimation. General standard techniques of genetic engineering – plasmid isolation, plasmid cloning, restriction enzyme etc.
6. Determination of optimum operational parameters and kinetic constants for enzyme reactions, immobilization techniques for enzymes and whole cell Estimation of kinetic parameters in microbial growth. \( K_a \) measurement in a bioreactor. Dissolved oxygen monitoring and control in bioreactor.
7. Production, recovery and control tests: alcohol, baker’s yeast, citric acid, enzymes, vitamins, amino acids, antibiotics, etc.
8. Biodegradation of organic compounds.

**Paper –VI (MChE–206): Project Seminar**

The candidate shall have to select a topic suitable for research or investigation, prepare a comprehensive review and critique of the work already done, carry out preliminary investigations and propose a plan of work. The candidate shall have to make a presentation of the report prepared, in a seminar.

**Semester III**
**Practical Papers**


Each student shall be required to carry out investigation on the assigned problem as given in Semester I. He/she shall submit three copies of progress report on his/her work. The candidate shall have to make a presentation of the report prepared in a seminar. The report will be evaluated based on the performance at the seminar, viva-voce and progress report by three examiners including guide.

**Semester IV**
**Practical Papers**


Each student shall be required to carry out investigation on the assigned problem as given in Semester I. He/she shall submit three copies of thesis on his/her work. The candidate shall have to make a presentation of the report prepared in a seminar. The examination shall include a viva-voice on the thesis.