TEACHING SCHEME AND COURSE CONTENTS

FOR

MASTER OF TECHNOLOGY

IN

CHEMICAL TECHNOLOGY

DEPARTMENT OF CHEMISTRY

NATIONAL INSTITUTE OF TECHNOLOGY HAMIRPUR (H.P.)
**Programme Objective:**

- To provide extensive teaching and training in industry-oriented chemical techniques including analytical instrumentation, modern chemical technologies and novel research materials/methods.

- To emphasize the importance of understanding the functioning mechanism of diverse characterization devices and their applicability in emergence of enhanced, selective detection technologies. Special focus will be given to the fields of chemical/engineering materials, electrochemical devices, advance polymer/composite platforms, spectroscopic tools and their applications.

- To provide students hand-on exposure on advanced instruments, cutting edge R&D and promote them for carrying out interdisciplinary works to address national/regional issues.

- To inculcate good communication skills, technical/scientific curiosity and knowledge among students via regular presentations, seminars, quizzes, and project discussions.

**Duration of the Programme:**

Two years (Four Semesters)

**Intake:**

Fifteen students (reservation as per GOI norms)

**Eligibility for admission:**

The applicant must have a Master Degree in Chemistry (with Physics and Mathematics at UG level) or Bachelor Degree in Chemical Engineering/Biotechnology/Material Science and Engineering with CGPI of 6.5 on a 10-point scale (or equivalent) or 60% marks in case of Open/OBC candidates in qualifying degree. Whereas in case of SC/ST candidates, a CGPI of 6.0 on a 10-Point scale (or equivalent) or 55% marks in qualifying degree will be applicable. The admission to M.Tech. programme will be as per institute norms.
### M. TECH. PROGRAMME IN CHEMICAL TECHNOLOGY
#### DEPARTMENT OF CHEMISTRY

#### SEMESTER-I

<table>
<thead>
<tr>
<th>Course No.</th>
<th>Subject</th>
<th>Teaching Schedule</th>
<th>Hours/Week</th>
<th>Credits</th>
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<tbody>
<tr>
<td>CH-600</td>
<td>Industrial Catalytic Processes</td>
<td>3 0 0</td>
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<tr>
<td>CH-601</td>
<td>Electroanalytical Chemistry</td>
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<td>CH-602</td>
<td>Advanced Transport Phenomena <em>(from Chemical Engineering Department)</em></td>
<td>3 0 0</td>
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<td></td>
<td>Programme Elective -I</td>
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<td>Programme Elective -II</td>
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<tr>
<td>CH-603</td>
<td>Electrochemical Techniques: Lab.</td>
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#### SEMESTER-II

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<td>CH-604</td>
<td>Industrial Chemical Technology</td>
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<tr>
<td>CH-605</td>
<td>Modern Spectroscopic Techniques and Instrumentation</td>
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<tr>
<td>CH-606</td>
<td>Chemical Reaction Engineering <em>(from Chemical Engineering Department)</em></td>
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<td></td>
<td>Programme Elective -III</td>
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<td>Open Elective-I <em>(from other Dept.)</em></td>
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<td>CH-607</td>
<td>Material Synthesis and Characterization Lab.</td>
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#### SEMESTER-III

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<tr>
<td>CH-799</td>
<td>Self Study</td>
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<td>CH-800</td>
<td>Seminar</td>
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<td>CH-801</td>
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#### SEMESTER-IV

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<td>CH-801</td>
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### Programme Elective Courses

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<tr>
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<th>Course Title</th>
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<tr>
<td>CH-700</td>
<td>Advanced Polymer Technology</td>
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<td>CH-701</td>
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<td>CH-702</td>
<td>Advanced Nanostructured Materials</td>
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<td>CH-703</td>
<td>Industrial Safety in Process Industries <em>(from Chemical Engineering Department)</em></td>
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<td>CH-704</td>
<td>Modern Materials Characterization Techniques</td>
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<td>CH-705</td>
<td>Environmental Chemical Technology</td>
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### Open Electives

(To be offered to the students from other Departments/Centres except Department of Chemistry)

(i) **CH-750** Composite Materials  
(ii) **CH-751** Molecular Modelling
Course Syllabus

CH-600: Industrial Catalytic Processes (Program core-1)
(3-0-0, 3 hours, 3 credits)

- **Catalysis and its Industrial Applications**: Homogeneous & heterogeneous catalysis; Role of catalytic processes in modern chemical manufacturing—catalysis in syngas manufacture, catalysis in organic polymer chemistry; catalysis in petroleum industry; catalysis in environmental control.
- **Enzyme Catalysis**: Transition states and enzyme catalysis; Enzymes in chemical biotransformations; Pre-steady state and steady state kinetics; Kinetics in industrial processes, Toxicological considerations and safety in handling enzymes; Enzyme immobilization and concept of protein and enzyme engineering, Applications of enzymes in industry and medicine, Enzyme inhibition.

Books and References:
2. Homogeneous transition metal catalysis – Christopher Masters

CH-601: Electroanalytical Chemistry (Program core-2)
(3-0-0, 3 hours, 3 credits)

Books and References:

CH-602: Advanced Transport Phenomena (Program core-3)
(3-0-0, 3 hours, 3 credits)
Summary of Vector and Tensor Notation: Vector operations from a geometrical view point, Vector operation from an analytical view point, the vector differential operations, second order tensors, vector and tensor components in curvilinear coordinates, differential operations in curvilinear coordinates.
Velocity Distributions in Laminar Flow: Shell momentum balances: boundary conditions, flow of a falling film, flow through a circular tube, flow through an annulus, adjacent flow of two immiscible fluids.
The Equations of Change for Isothermal Systems: Equation of continuity, the equation of motion, the equation of mechanical energy.
The Equations of change for Non isothermal systems: The equations of energy, the energy equation in curvilinear coordinates, the equations of motion for forced and free convection in non-
isothermal flow, summary of the equations of change, use of equation of change to set up steady-state heat transfer problems.

**Diffusivity and the Mechanism of Mass Transport:** Definition of concentrations, velocities and mass fluxes, fick’s law of diffusion, theory of ordinary diffusion in gases at low density, theory of ordinary diffusion in liquids.

**Concentration Distributions in Solid and in Laminar Flow:** Shell mass balances: boundary conditions, diffusion through a stagnant gas film, diffusion with heterogeneous chemical reaction, diffusion with homogeneous chemical reaction, diffusion into a falling liquid film, forced – convection mass transfer, Analogies between Heat, mass and momentum transfers.

**Books and References:**


**CH-603: Electrochemical Techniques: Lab.**

*(3-0-0, 3 hours, 2 credits)*

Use of Conductometry /Potentiometry in understanding precipitation reactions, inorganic complex formations, determination of kinetic parameters of chemical reactions, and micelle formation in soap solutions. Electrochemical estimation of dissociation constant of amino acids. Practical verification of electrochemical Tafel equation. Determination of amount of metal ions in samples using polarography.

**Books and References:**


**CH-604: Industrial Chemical Technology (Program core-4)**

*(3-0-0, 3 hours, 3 credits)*

**Dyes:** Structure and properties, Natural colours/dyes for textile applications, Natural food colours and their health aspects, Biomedical applications of dyes: Photodynamic therapy, Dyes in
bioanalysis and medical diagnostics, DNA sequencing, Cancer detection, activity with diazonium salts, Dyes as therapeutic agents.

**Sugar Technology:** Introduction to sugar industry, Specification of raw sugar, Refining quality of raw sugar – evaluation, calculation of raw value, By-products and co-products of sugar industry

**Chemistry of Food Preservatives:** Objectives and techniques of food preservation; Structure, properties and use of foods preservative: chemical preservative, biopreservative including antibiotics.

**Petrochemicals – Structure, Properties and Applications:** Types of crude oil, Properties of Petroleum oil products: Definition and significance of various properties like API gravity, Aniline point, Diesel index, Cloud point, Pour point, Flash point, Fire point, Smoke point, Octane number, Cetane number, Softening point; Manufacturing process of Chemicals from methane: synthesis of methanol, Acetic acid, Vinyl Acetate, Poly Vinyl Acetate, Specific requirements for automotive lubricants, oxidation deterioration and degradation of lubricants, additives and additive mechanism, synthetic lubricants.

**Books and References:**
1. Functional Dyes, S H Kim, Elsevier BV 2006
3. Natural Dyes and their Applications in Textiles by M. L. Gulrajani, IIT Delhi
4. Natural Food Colorants by Gabriel J. Lauro and F. Jack Francis (eds), Marcel Dekker Inc.
5. Manufacture and Refining of Raw Cane Sugar – V E Baikow
6. Industrial Utilisation of Sugarcane & Its Co-products - P J Manohar Rao
7. Technology of Food Preservation by Desrosier

**CH-605: Modern Spectroscopic Techniques and Instrumentation (Program core-5)**

(3-0-0, 3 hours, 3 credits)

UV-Visible spectroscopy; Vibrational Spectroscopies (Raman, FTIR, SFG); NMR as characterization tool: instrumentation, recent advances and analytical applications; Mass spectrometry and its applications; Atomic absorption and emission spectrometry; Fluorescence and phosphorescence based methods; Chromatographic methods of separation; Gas chromatography and HPLC.

**Books and References:**
CH-606: Chemical Reaction Engineering (Program core-6)

(3-0-0, 3 hours, 3 credits)

**Introduction:** Kinetics of homogeneous chemical and biochemical reactions, single and multiple reactions, order & molecularity, rate constant, elementary and non elementary reactions, temperature dependent term of rate equation, Constant volume batch reactor, integral method of analysis of data, series and parallel reactions, reversible reactions, Variable volume batch reactor, Differential methods of analysis, Temperature and reactions rate; Types of Microorganisms: Structure and function of microbial cells; Fundamental of microbial growth; batch and continuous culture; Isolation and purification Enzymes from cells; Assay of Enzymes; Metabolism and bio-energetics.

**Reactors:** Fixed Bed Catalytic Reactor, Single and multi bed adiabatic reactors, Multi tubular fixed bed reactor. Kinetic Regimes for Mass Transfer and Reaction, Film Conversion parameter, Clues to the kinetic Regime from solubility data, Clues to the Kinetic Regime from equipment, Applications to design, Reactor Design and Analysis for soluble enzyme systems.

**Bio Reactors — Effect of Transport Processes:** Introduction to Bioreactor design: Continuously Stirred aerated tank bioreactors. Mixing power correlation; Determination of volumetric mass transfer rate of oxygen from air bubbles and effect of mechanical mixing and aeration on oxygen transfer rate, heat transfer and power consumption; Multiphase bioreactors and their applications; Downstream processing and product recovery in bioprocesses.

**Rate Equations for Fluid solid catalytic reactions:** Rates of Adsorption, Surface reaction, Desorption, Rate limiting step, Power Law, Langmuir Hinshelwood rate, Eley Rideal mechanism, Packed bed reactor and fluidized bed reactor, Numerical Problems.

Books and References:

(3-0-0, 3 hours, 2 credits)
Single and double stage preparation of organic/inorganic/polymeric materials; purification using column chromatography, thin layer chromatography, Flash chromatography, GC, HPLC, Identification and Characterization of the same using UV, FTIR, NMR (1D, 2D, 3D), Raman, X-ray diffraction and mass spectroscopic techniques.

Books and References:
2. Advanced Practical Organic Chemistry by N.K. Vishnoi
3. Organic Spectroscopy by W. Kemp

Program Electives
CH-700: Advanced Polymer Technology
(3-0-0, 3 hours, 3 credits)
Introduction: Molecular weight distribution, glass transition, morphology, viscosity vs. molecular weight and mechanical property vs. molecular weight relationships, Methods of determination of molecular weight, distribution, size and shape of macromolecules, Mark-Houwink relationship, Thermodynamics of polymer solutions, Rubber elasticity concepts, thermodynamic equation of state.
Polymerization Techniques- bulk, solution, emulsion-description of the process, progress of polymerization, rate of polymerization, degree of polymerization, suspension, living radical polymerization technique, Mechanical properties of polymers and methods of determination, selected commercial polymers and applications.
Polymer modifications and recent technological advances toward live cell encapsulation and delivery, Surface modification of natural fibers for reinforcement in polymeric composites, Biopolymers based stimuli-sensitive functionalized graft copolymers as controlled drug delivery systems.

Role of polymers for high-tech areas such as light emitting diode, OSR in satellite communication, photovoltaic etc., High temperature polymers such as polyimides, polyetherimides, PEEK, silicone etc., their preparations, properties & applications, Liquid Crystalline polymers- their synthesis, properties and applications, High energy absorbing polymer, Super absorbent polymers - their synthesis, properties and applications.

Books and References:
7. Polymer Science and Technology by J. R. Fried.

CH-701: Numerical & Computational Methods in Chemical Engineering
(3-0-0, 3 hours, 3 credits)
Treatment of engineering data-graphical representation, empirical equations, Interpolation; Newton’s formula, Lagrange’s interpolation formula, extrapolation, integration, graphical Integration, graphical construction of integral curves, numerical integration.
Interpretation of Engineering Data- significant figure, classification of measurements, propagation of errors, variation and distribution of random errors, properties of variance, confidence limits for small samples.
Numerical Solutions of Ordinary Differential Equations – linear second–order equations with variable coefficients, numerical solution by Runge kutta method. its application to higher–order equations
Formulation of partial differential equations, finite difference, linear finite difference equations, non-linear difference equations, optimization, types of methods, its application relating to chemical
processes.

Books and References:
1. Applied Mathematics in Chemical Engineering, Mickley HS, Sherwood and Reed, TMH pub.
2. Mathematical Methods in Chemical Engineering, Jenson & Jeffrey’s, McGraw Hill

CH-702: Advanced Nanostructured Materials
(3-0-0, 3 hours, 3 credits)
Introduction; fundamentals of colloidal chemistry; Synthesis, preparation and fabrication: chemical routes, self assembly methods, biomimetic and electrochemical approaches; Size controls properties (optical, electronic and magnetic properties of materials) - Applications (carbon nanotubes and nanoporous zeolites; Quantum Dots, basic ideas of nanodevices).

Books and References:
2. Nanostructures & nanomaterials: synthesis, properties & applications, by Guozhong Cao, Imperial College Press, London
3. Introduction to nanoscience and nanotechnology, by Gabor L. Hornyak, Harry F. Tibba et.al., CRC Press, New York

CH-703: Industrial Safety in Process Industries
(3-0-0, 3 hours, 3 credits)
Introduction: Industrial safety principles, Site selection and plant layout, Legal Aspects, Design for ventilation, Emergency response systems for hazardous goods basic rules and requirements which governs the chemical industries.

Hazards: Chemical hazards classification, Hazards due to fire, explosion and radiation, Reduction of process hazards by plant condition monitoring, Materials Safety Data sheets and National Fire protection agency's classifications.

Diseases: Dangerous occupational diseases, poisoning, dust effect, Biomedical and engineering response to health hazards.

Control of Hazards: Engineering control of plants instrumentation, Color codes for pipe lines, Safety aspects of reactive chemicals.


Hazard identification: Hazard survey, checklist, HAZOP, safety reviews
Risk Assessment: Probability theory, event tree, fault tree, QRA and LOPA, Dow’s fire and explosion index, Mond index, Dow’s Chemical release model

Case Histories: Accident Investigations: Bhopal gas tragedy, flixborough disaster, Pasadena accident, IOCL disaster

Books and References:

CH-704: Modern Materials Characterization Techniques
(3-0-0, 3 hours, 3 credits)
Mechanical Testing of materials; Thermal analysis techniques: TGA, DTA & DSC; Magneto-Optical Characterization of Magnetic Thin Films, Surfaces, and Interfaces at Small Length and Short Timescales; Basic concepts of diffraction techniques (powder and single crystal) for inorganic, organic and hybrid materials; Applications of electron microscopic techniques (scanning and transmission) for morphological and nanostructural features; Scanning Probe Microscopies (STM, AFM, SNOM), Photoelectron Spectroscopy: XPS and Auger.

Books and References:
1. Characterization of Materials, Elton N. Kaufmann (Ed.)
3. Characterization of Materials by P.K. Mitra

CH-705: Environmental Chemical Technology
(3-0-0, 3 hours, 3 credits)
- Water and waste water analysis: Determination of acidity/alkalinity, turbidity, hardness, residual chlorine, BOD, COD and other inorganic/organic contaminants.
- Chemical Toxicology: Dose-response relationships, toxicology of metal ions, pesticides, insecticides and food additives.
- Waste management and application of Green technology
- Industrial pollution and its control by application of biotechnology, Radioactive wastes and their proper disposal, Pollution from agrochemicals and its control.
INTERNATIONAL STANDARD ISO 14040: Environmental management - Life cycle assessment - Principles and framework

Books and References:
2. Environmental Chemistry with Green Chemistry by A.K. Das and M. Das
3. INTERNATIONAL STANDARD ISO 14040

Open Elective

CH-750: Composite Materials
(3-0-0, 3 hours, 3 credits)
Introduction to composite materials, comparison of different materials with composites- advantages and disadvantages, Principles of composite reinforcement, Effect of fibrous reinforcement on composite strength, Types of reinforcement such as natural, glasses, carbon/graphite, aramid fiber, high strength and high modulus fibers, Surface treatment and various forms of fibers. Processing and production techniques like hand-layup, bag moulding, filament winding, pultrusion, Prepeg, their manufacture and characterization, Sheet moulding and dough moulding compounds and their processing, resin transfer mouldings. Application of self reinforced composites, Concept of nanofillers and polymer nanocomposites, Surface modification of cellulose nanocrystals for nanocomposites, Surface modification of natural fiber composites and their potential applications.

Books and References:
3. Hand Book of Fibre glass and Advanced Plastic Composites, by G. Lubin

CH-751: Molecular Modelling
(3-0-0, 3 hours, 3 credits)
Molecular Mechanics, Simulation of Molecular Ensembles, Foundation of molecular orbital theory, Semi-empirical implementations of molecular orbital theory, Ab initio implementations of Hartee-Fock molecular orbital theory, Density Functional Theory, Charge Distribution and Spectroscopic
properties, Thermodynamic properties, Hybrid quantal/classical models, Gaussian Techniques, Docking, 2D and 3D QSAR, Applications in pharmaceutical industry and designing of new varieties of polymers/pesticides/pigments/materials.

**Books and References:**

2. Molecular Modelling: Principles and Applications, by Andrew Leach