Vidyasagar University

Curriculum for Industrial Chemistry (Major)

[Choice Based Credit System]

Semester-V

Course	Course Code	Name of the Subjects	Course Type/ Nature	Teaching Scheme in hour per week			Credit	Marks
				L	T	P		
CC- 11		**C11T:** Advanced Numerical Analysis and Advanced Reaction kinetics	Core Course-11	4	0	0	6	75
		C11P: Cement Testing Lab		0	0	4		
CC- 12		**C12T**: Petroleum Chemistry	Core Course-12	4	0	0	6	75
		C12P: Fuels & Furnace Lab		0	0	4		
DSE-1		**TBD**	Discipline Specific Elective - 1	5	0	1	6	75
DSE-2		**TBD**	Discipline Specific Elective - 2	5/4	1/0	0/4	6	75
Semester Total							**24**	**300**

L= Lecture, **T=** Tutorial, **P =** Practical, **CC -** Core Course, **TBD -** To be decided, **DSE:** Discipline Specific Elective.

SEMESTER- V

List of Core Course (CC)

CC-11: Advanced Numerical Analysis and Advanced Reaction kinetics

CC-12: Petroleum Chemistry

Discipline Specific Electives (DSE)

DSE-1: Green Chemistry

Or

DSE-1: Concept of heavy Inorganic Chemicals & petrochemicals & Industrial and Environmental pollution

DSE-2: Analytical methods in Chemistry

Or

DSE-2: Molecular Spectroscopy, Material Science and Metallurgy

Core Course (CC)

CC-11: Advanced Numerical Analysis and Advanced Reaction kinetics **Credits 06**

C11T : Advanced Numerical Analysis and Advanced Reaction kinetics **Credits 04**

Course Contents:

Unit-I : Advanced Numerical Analysis **(Marks 25)**

Data acquisition and processing:

Interpolation: Finite differences; Newton's forward and backward interpolation formula; Lagrange's formula; Central differences; Formula of Gauss, Bessel and Everett curve fitting: Method of least squares; Cubic splines.

Solution of algebraic and transcendental equations: Iterative methods, Newton-Raphson method, convergence and efficiency of method.

Matrices: Eigen value and Eigen vectors, matrix decomposition, inverse of matrix, norm of matrix.

Solution of System of Linear equations: Direct methods: Gauss elimination method, LU – Decomposition, Cholesky method, iteration methods: Jacobi method, Gauss- Seidel method; Ill conditioned systems. Numerical integration and differentiation.

Numerical solution of ordinary differential equations: Euler method, Modified Euler method and Runge-Kutta method.

Finite difference method for solution of boundary value problems of ordinary and partial differential equations.

Unit – II: Advanced Reaction kinetics **(Marks 25)**

Fundamental aspects of Reaction Kinetics, Collision and Transition state theories of reactions rates. Kinetics of homogeneous and heterogeneous catalytic reactions. Kinetics of electrochemical reactions with special reference to hydrogen evolution reaction and electrodeposition.

Complex reactions; Mechanism of complex reaction, derivation of differential rate equations, steady state and rate limiting approximations as applied for complex reactions, fast reactions, techniques for study of fast reactions. Explosion reactions. Ionic chain reactions; Mechanism of ionic chain reactions and their kinetics. Kinetic treatment of diffusion in solids, liquids and solutions.

C11P: Cement testing Laboratory **Credits 02**

Practical **(Marks 25)**

a) Estimation of Lime by Rapid Lime Method, Total Carbonate of Sample, Full analysis (SiO_2, Al_2O_3, Fe_2O_3, CaO and MgO) of Cement & Clinker.

b) Physical testing of Cement: Compressive testing, Specific surface area analysis etc.

Suggested Books/ Reading:

1. S. S. Sastry: Numerical Analysis, Prentice Hall of India Pvt. Ltd., New Delhi.
2. M. K. Jain; Numerical Methods for Scientists and Engineers et. al., New Age International Publishers, New Delhi.
3. K.J. Laidler: Chemical Kinetics, 3rd Ed. Pearson Education Inc.
4. J. Rajaram, J.C. Kuriacose: Kinetics and Mechanisms of Chemical Transformations, McMillan. India Ltd.
5. S.K. Upadhayay: Chemical Kinetics and Reaction Dynamics, Anamaya Publishers, New Delhi
6. J.O'M. Bockris and A.K.N. Reddy: Modern Electrochemistry Vol II, Plenum Press, and New York.

CC- 12: Petroleum Chemistry **Credits 06**

C12T: Petroleum Chemistry (Marks 50) **Credits 04**

Course Contents:

Unit-I : Composition of Petroleum

Introduction to crude oil, exploratory methods, oil reservoirs, Evaluation of oil stocks, Physical properties of a petroleum oil- Specific Heat, Latent Heat, Critical point & other properties, coefficient of Expansion, Detonation Characteristics.

Unit-II : Introduction to processing and Refinery Products

Refinery and Distillation Processes : Boiling Range of Stock, Arrangement of Towers, Flow diagram and operating conditions, Vacuum distillation, Desulphurisation, Refining by adsorption, Preliminary ideas of treating equipments and extraction processes, Dewaxing.

Unit-III: Meaning of the important terms

Meaning of terms such as - Pour point depressants, drag reducers, viscosity reducers, ignition point, flash point, octane number, doctor solution types of hydrocarbon fuels and their characteristics.

Unit-IV: Basic operations in petrochemical industry

Basic idea about the following operations with respect to process, mechanism, catalysts used and applications: Cracking - Catalytic cracking, Hydrocracking, Isomerization, Reforming, Isomerization, Alkylation. Sulphur, hydrogen, petroleum coke and nitrogen compounds from petroleum.
Various catalysts used in petrochemical industry, preparation structure, applications and selectivity.

C12P: Fuels & Furnace Lab (Marks 25) Credits 02

Course Contents:

Determination of Fire Point, cloud point, pour point, Kinetic Viscosity of oil, Proximate analysis of coal, Calorific value of Solid Fuel.

Discipline Specific Electives (DSE)

DSE-1: Green Chemistry Credits 06

DSE1T: Green Chemistry (Marks 75) Credits 06

Course Contents:

Unit-I: Introduction to Green Chemistry:

What is Green Chemistry? Some important environmental laws, pollution prevention Act of 1990, emergence of green chemistry, Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

Unit-II: Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry and their explanation with examples *Special emphasis on the following:*

- Designing a Green Synthesis using these principles; Prevention of Waste/ by products; maximum incorporation of the materials used in the process into the final products , Environmental impact factor
- Green metrics to assess greenness of a reaction, e.g. Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
- Prevention/ minimization of hazardous/ toxic products reducing toxicity
- Risk = (function) hazard x exposure; waste or pollution prevention hierarchy
- Designing safer chemicals with minimum toxicity yet has the ability to perform the desired functions

- Green solvents: super critical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, solvents obtained from renewable resources and how to compare greenness of solvents
- Energy requirements for reactions – alternative sources of energy: use of microwaves, ultrasonic energy and photochemical energy
- Selection of starting materials; should be renewable rather than depleting
- Avoidance of unnecessary derivatization – careful use of blocking/protecting groups
- Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, bio catalysis, asymmetric catalysis and photo catalysis.
- Design for degradation: A product should not persist after the commercial function is over e.g. soaps and detergents and some more
- Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.
- Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD "What you don't have cannot harm you", greener alternative to Bhopal Gas Tragedy (safer route o carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.

Unit-III: Examples of Green Synthesis/ Reactions

- Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)
- Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents, Diels-Alder reaction and Decarboxylation reaction
- Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)

Unit-IV: Real world case studies based on the Presidential green chemistry awards of EPA

- Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments.
- A new generation of environmentally advanced wood preservatives: Getting the chromium and Arsenic out of pressure treated wood.
- An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.
- Healthier Fats and oils by Green Chemistry: Enzymatic Inter esterification for production of No Trans-Fats and Oils.
- Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting.
- Using a naturally occurring protein to stimulate plant growth, improve crop quality, increase yields, and suppress disease.

Unit-V: Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimcry and green chemistry, biomimetic, multifunctional reagents, combinatorial green chemistry, mechanochemical and solvent free synthesis of inorganic complexes; co crystal controlled solid state synthesis (C^2S^3); Green chemistry in sustainable development.

Suggested Books/ Readings

- P.T. Anastas & J. C. Warner, Green Chemistry, Theory and Practice, Oxford University Press (1998).
- M. Lancaster , Green Chemistry An Introductory Text. RSC Publishing, 2nd Edition. ISBN: 978-1-84755-873-2 (2016).
- M. C. Cann & M. E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
- M. C. Cann and ,Thomas P Umile, Real world cases in Green chemistry vol 11, American chemical Society,Washington (2008)
- A.S. Matlack, Introduction to Green Chemistry, Marcel Dekker (2001).
- V. K. Alhuwalia and M.R. Kidwai,New Trends in Green chemistry, Anamalaya Publishers (2005)
- A. L Garay, A. Pichon and S.L. James, Chem Soc Rev, 36,846-855 (2007).
- http// Biomimicry.org/askingnature
- Janine Benyus: Innovations Inspired by nature,Harper collins 1997

Or

DSE-1: Concept of Heavy Inorganic Chemicals & petrochemicals & Industrial & Environmental pollution

Credits 06

DSE1T: Concept of Heavy Inorganic Chemicals & petrochemicals & Industrial & Environmental pollution (Marks 75)

Credits 06

Course Contents:

Unit-I: Heavy Inorganic chemicals:

i) Manufacture of Sulphuric Acid, Hydrochloric acid, Nitric acid, Phosphoric acid.

ii) Fertilizer Industries: Phosphorus Fertilizers - phosphorus, phosphoric acid, ammonium phosphate, superphosphate, triple superphosphate, Nitrogen Fertilizers - Urea, other fertilizers like ammonium nitrate and ammonium sulphate. Inorganic disinfectant chemicals.

Note: Physico-Chemical Principles, Major equipment's, material of construction to be emphasized in the entire above topic.

Unit-II: Petrochemicals:

Crackers-isolation of different chemicals:

i) C_1 chemicals: Methanol, Formaldehyde, Chlorinated Methanes.

ii) C_2 ,C_3 and C_4 chemicals: Ethyl Chloride, Vinyl Chloride, Ethylene oxide, Ethylene Glycol, Ethanolamines, Acetaldehyde, Acetic acid, Isopropanol, Oxo-synthesis, Acrylonitrile.

iii) Aromatic compounds- Production and isolation of BTX, monobasic and di-basic acid and its ester, Styrene, Napthalene, Linear Alkyl Benzenes and their sulphonates.

Basic Drugs such as Anti-malarials, Anti-amoebic, Analgesic and Anti-pyretic, Broad Spectrum Anti-biotics -Ampicillin, Chloromycetin.

Unit-III: Industrial & Environmental pollution

Industrial & Environmental pollution - An overview: Pollution and pollutants-sources, types and consequences. Air and Water pollution, solid wastes. Imbalance in atmosphere, Hydrosphere and Lithosphere. Industrial Effluents. Industrial Episodes of hazards and pollution: Minamata, Love canal, Flixborough, Bhopal, Chernobyl.

Water as Environmental Resources: Hydrological cycle. Water quality, criteria of pollution suspended solids; physical chemical and biological; dissoloved solids-organics, Bio-degradable and Nonbiodegradable; Inorganic heavy metal and others.

Assessment of water quality- sampling and analysis- Dissoloved oxygen(DO), Bio- chemical oxygen demand (BOD), Chemical oxygen demand(COD), Industrial methods for total organic carbon (TOC), Colorimetric and gas chromatographic methods; Analysis of toxic inorganic pollutants- as fluoride, Hg, Cd, Pb, Sb, Coliform test.

Drinking water standards (India and WHO), Industrial discharge Standards -Minimum National Standards (MINAS)

Waste water treatment methods: Physical, chemical and biological , Primary, secondary and tertiary, Removal of Biodegradable Organics- Activated Sludge Methods , Fixed Film methods- Trickling Filter, Rotating Biological Contractor (RBC), Design criteria of Bio- reactor, Pond Treatment and soil treatment systems. Bioremediation. Concepts of recycling and zero discharge industries.

Air composition and quality: Chemical and photochemical reactions in the atmosphere. Ozone formation and depletion, green house effect.

DSE- 2: Analytical Methods in Chemistry Credits 06

DSE2T: Analytical Methods in Chemistry (Marks 50) Credits 04

Course Contents:

Unit I: Qualitative and quantitative aspects of analysis

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression.

Normal law of distribution of indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

Unit II: Optical methods of analysis

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules.
UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument; Transmittance. Absorbance and Lambert-Beer law.
Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers.
Flame Atomic Absorption and Emission Spectrometry:
Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

Unit III: Thermal methods of analysis

Theory of thermogravimetry (TG), basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture.

Unit IV: Electroanalytical methods

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations.
Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values.

Unit V: Separation techniques

Solvent extraction:
Classification, principle and efficiency of the technique.
Mechanism of extraction: extraction by solvation and chelation, Technique of extraction: batch, continuous and counter current extractions, Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and non-aqueous media.
Chromatography:
Classification, principle and efficiency of the technique, Mechanism of separation: adsorption, partition & ion exchange, Development of chromatograms: frontal, elution and displacement methods.

DSE2P: Analytical Methods in Chemistry (Practical) (Marks 25) Credits 02

List of Practical

I. Separation Techniques

Chromatography:

(a) Separation of mixtures

(i) Paper chromatographic separation of Co^{2+} and Ni^{2+}.

(ii) Separation and identification of the amino acids present in the given mixture by paper chromatography. Reporting the R_f values.

II. Solvent Extractions:

(i) To separate a mixture of Ni^{2+}& Fe^{2+} by complexation with DMG and extracting the Ni^{2+} DMG complex in chloroform, and determine its concentration by spectrophotometry.

III. Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

(iii) Estimation of calcium, magnesium

(iv) Qualitative detection of nitrate, phosphate

IV. Ion exchange:

(i) Determination of exchange capacity of cation exchange resins and anion exchange resins.

(ii) Separation of amino acids from organic acids by ion exchange chromatography.

Spectrophotometry

Verification of Lambert-Beer's law and determination of concentration of a colored species ($CuSO_4$, $KMnO_4$)

Suggested Books/ Readings

Theory:

- Vogel, Arthur I: A Text book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5 th Ed. The English Language Book Society of Longman .
- Willard, Hobart H. et al.: Instrumental Methods of Analysis, 7 th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6 th Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A., Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore, 1998.

- Mikes, O. and Chalmers, R.A. Ed. Laboratory Hand Book of Chromatographic and Allied Methods, Elles Horwood Ltd. London.
- Dilts, R.V. Analytical Chemistry – Methods of separation Van Nostrand 1974

Practical:

- Vogel, Arthur I: *A Text book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Willard, Hobart H. et al.: *Instrumental Methods of Analysis, 7th Ed*. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; *Analytical Chemistry, 6th Ed*. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. and Nieman, T.A. *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore, 1998.
- Mikes, O. & Chalmers, R.A. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Horwood Ltd. London.

Or

DSE-2: Molecular Spectroscopy, Material Sc. and Metallurgy Credits 06

DSE2T: Molecular Spectroscopy, Material Sc. and Metallurgy (Marks- 75) Credits 06

Course Contents:

Unit 1: Molecular Spectroscopy

I. Light-matter interaction, transition moment integral, selection rule, Spectroscopic arrangements.

II. Rotational spectroscopy of diatomic molecules: rigid rotor model, selection rules, spectrum, characteristicfeatures of spectral lines (spacing and intensity). Determination of bond length, effect of isotopic substitution.

III. Vibrational spectroscopy of diatomic molecules: SHO model, selection rule, spectra; anharmonicity and its consequences on energy levels, overtones, hot bands, Raman Effect. Characteristic features and condition of Raman activity with suitable illustraitons. Rotational and vibrational Raman spectra. Rule of mutual exclusion with examples.

IV. Potential energy curves (diatomic molecules), Decay of excited states by radiative and non-radiative paths. Fluorescence and phosphorescence, Jablonsky diagram.

Unit 2: Materials Science

1. Introduction of Material Science and Engineering, Classification of materials, Introduction to engineering materials, Materials Design and selection, advanced materials.

2. Structure of crystalline solid: lattice, basis, unit cell, crystal system, point coordinates, crystallographic direction, crystallographic plane. Concept of amorphous, single crystalline and poly crystalline material. Radius ratio rule, Crystal structures of ionic materials. Structural analysis and phase identification using X-ray diffraction technique. Crystal imperfections: point defects, linear defects, surface defects & importance of defects.

Unit 3: Metallurgy

a) Basic divisions: Pyrometallurgy, hydrometallurgy and electrometallurgy, basic metallurgical operations -Pulverisation ,Calcination, Roasting , Refining, Smelting.
b) Meatllurical thermodynamics: Application of thermodynamics in metallurgy. Ellingham and kellog diagram. Gibb's phase rule, Iron Carbon equilibrium diagram for eutectoid and pro-eutectoid phases. Lever rule. Nature of cooling curves for Fe-C system.
c) Physico-chemical principles & details of extraction as per Indian context of the following metals; Copper, Lead, Silver, Aluminium, Zinc.
d) Production of Iron in blast furnace-Raw materials, charging and sequence of operations, casting,operation of pig casting machine.
e) Production of semi-killed and killed steel in steel melting shop (LD process)- mixing of raw materials, charging sequences, operation in converter, blowing, tapping and testing process, timing in pit side, holding and stripping operations.
f) Continuous casting of semi-finished steel products.

Suggested Books/ Readings

Molecular Spectroscopy

a) Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).
b) Fundamentals of Molecular Spectroscopy by P.S. Sindhu, New Age International Publishers.
c) Introduction to MOLECULAR SPECTROSCOPY by G.M BARROW, McGraw-Hill.
d) Molecular Spectroscopy by J.L. McHale, CRC Press, Taylor & Francis Group.

Materials Science

1. Material Science & Engineering – William D. Callister, Jr.
2. Material Science & Engineering – V. Raghaban, prentice hall of India Pvt Ltd.
3. Essentials of Material Science & Engineering – Donald R. Askeland, pradeep P. Fulay.

Metallurgy

1. Extraction of Nonferrous Metals- H.S.Ray, R. Sridhar, K.P. Abraham, Affiliated East- West Press Pvt. Ltd., New Delhi.
2. Principles of Extractive Metallurgy- H.S. roy and A. Ghosh - New Age International (P) Ltd., Publishers, New Delhi.

3. Engineering Chemistry- P.C. Jain & Moni Jain, Dhanpat Rai PublishningCo.P. Ltd., New Delhi.
4. Industrial Chemistry- B.K.Sharma, Geol Publishing house, Meerut-25001,U.P

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