Scheme for B. Tech. Chemical Engineering with Honors

S. No.	Course Code	Course Title	Semester	Type	Credit	L	T	P
1.	22CHT303	Heterogeneous Catalysis	V	Theory	3	3	0	0
2.	22CHT309	Soft Matter	V	Theory	3	3	0	0
3.	22CHT357	Process Intensification	VI	Theory	3	3	0	0
4.	22CHT352	Multiphase Reactors	VI	Theory	3	3	0	0
5.	22CHT402	Molecular Modeling of Chemical Systems	VII	Theory	3	3	0	0
6.	22CHT452	Process Industry 4.0	VIII	Theory	3	3	0	0
Total					**18**	**18**	**0**	**0**

B. Tech. Chemical Engineering with Honors

1. Subject Code: 22CHT303 **Course Title: Heterogeneous Catalysis**

2. Contact Hours: L: 3 T: 0 P: 0

3. Credits: 3 Semester: V

4. Pre-requisite: Nil.

5. Course Objective: To gain knowledge of heterogeneous catalysis, mechanism of catalytic reactions, and design of catalytic reactors.

6. Course Outcomes: On successful completion of the course students will be able to:

i. Develop various catalytic reaction mechanisms.
ii. Characterize a catalyst.
iii. Assess the effects of external heat and mass transfer effects in heterogeneous catalysis.
iv. Calculate the effectiveness of a porous catalyst.
v. Design different types of reactors for catalytic reactions.

7. Details of Course:

Unit No.	Contents	Contact Hours
1.	Heterogeneous Catalysis, Analysis of external transport processes in heterogeneous reactions in fixed bed, fluidized bed and slurry reactors. Intra-pellet mass transfer, heat transfer, mass transfer with chemical reaction and simultaneous mass and heat transfer with chemical reaction.	10
2	Catalyst Selectivity: Effect of intra-pellet diffusion on selectivities in complex reactions, effect of external mass transfer on selectivities.	10
3	Catalyst Deactivation: Modes of deactivation – poisoning, fouling and sintering. Determination of deactivation routes, combined effect of deactivation and diffusion on reaction rates, effect of deactivation on selectivity.	10
4	Reactor Design: Design calculation for ideal catalytic reactor operating at isothermal, adiabatic and non-adiabatic conditions. Deviations from ideal reactor performance. Design of industrial fixed-bed, fluidized bed and slurry reactors. Thermal stability of packed bed and fluidized bed reactors.	10

8. Books:

(A) Text Books

S.No.	Authors / Name of Book / Publisher	Year of Publication
1.	Smith, J. M., "Chemical Engineering Kinetics," 3rd Ed., McGraw-Hill.	1981
2	Carberry, J. J., "Catalytic Reaction Engineering," McGraw-Hill.	1977

(B) Reference Books

S. No.	Authors / Name of Book / Publisher	Year of Publication
1	Denbigh, K.G., and Turner, J.C.R., Chemical Reactor Theory: An Introduction, Cambridge University Press.	1984
2	Carberry, J.J., Chemical and Catalytic Reaction Engineering, McGraw-Hill.	2001

1. Subject Code: 22CHT309 **Course Title: Soft Matter**

2. Contact Hours: L: 3 T: 0 P: 0

3. Credits: 3 Semester: V

4. Pre-requisite: Nil.

5.Course Objective: The course aims to describe the fundamental physics behind different soft materials, theirproperties, and applications in modern technologies.

6. Course Outcomes: On successful completion of the course students will be able to:

i. Understand how different kinds of matter are described mathematically and how material properties can be predicted based on microscopic structure and application of physical principles.

ii. Learn the importance of different soft materials in a variety of applications.

iii. Explain how different technological devices function

7. Details of Course:

Unit No.	Contents	Contact Hours
1.	Introduction: Intermolecular interactions, Structural organization, dynamics, phase transitions, order parameters, scaling laws, poly-dispersity, experimental techniques for investigating soft matter, computer simulation.	8
2.	Polymers: Introduction, synthesis, polymer chain conformation, characterization, polymer solutions, amorphous polymers, crystalline polymers, plastics, rubber, fibers, polymer blends and block copolymers, biopolymers.	8
3	Colloids: Introduction, types of colloids, forces between colloidal particles, characterization of colloids, charge stabilization, steric stabilization, effect of polymers on colloidal stability, kinetic properties, sols, gels, clays, foams, emulsions, food colloids, concentrated colloidal dispersions.	8
4	Amphiphiles : Introduction, types of Amphiphiles, surface activity, surfactant monolayers and Langmuir-Blodgett films, adsorption at solid interfaces, micellization and the critical micelle concentration, detergency, solubilization in micelles, interfacial curvature and its relationship to molecular structure, liquid crystal phases at high concentrations, membranes, templated structures.	8
5	Liquid crystals: Introduction, types of liquid crystals, characteristics of liquid crystal phases, identification of liquid crystal phases, orientational order, elastic properties, phase transitions in liquid crystals, application of liquid crystals.	8

8. Books:

(A) Text Books

S. No.	Authors / Name of Book / Publisher	Year of Publication
1.	Hamley I. W. "Introduction to Soft Matter", John Wiley & Sons Ltd.	2000

(B) Reference Books

S. No.	Authors / Name of Book / Publisher	Year of Publication
1	R.A.L. Jones. " Soft Condensed Matter", Oxford University Press	2004

1. Subject Code: 22CHT357 Course Title: Process Intensification

2. Contact Hours: L: 3 T: 0 P: 0

3. Credits: 3 Semester: VI

4. Pre-requisite: Nil.

5. Course Objective: The course will focus on the working and application of intensified equipments and techniques that potentially lead to compact, safe, energy-efficient, and environment-friendly sustainable processes.

6. Course Outcomes: On successful completion of the course students will be able to:

i. To understand the need of intensification of a process.
ii. To know methods of PI.
iii. To study and gain knowledge about different PI equipments in reaction and separation.
iv. Ability to model hybrid processes

7. Details of Course:

Unit No.	Contents	Contact Hours
1.	**Concept of Process Intensification (PI):** History, Philosophy, Principles, Definition, Need of process intensification **Ways of PI**: Process Intensifying Equipment, Process Intensifying Equipments, Examples of their application on the commercial scale.	6
2.	**Rotating Equipments**: Use of high gravity fields, HiGee Reactor, Spinning Disc Reactor. **Micro-concept Equipments**: Principles, Micro-reactors, Micro-channel heat exchangers, Monolithic catalyst and reactors.	12
3	**Reactive and Hybrid Separations**: Concept and principle, Distillation, Extraction, Precipitation, Adsorption, Absorption, and Fermentation-pervaporation, Adsorptive distillation, Membrance absorption and stripping.	10
4	**Multifunctional Reactors**: Principles, Integration of reaction, heat and mass transfer, Reverse flow reactor, Reverse flow reactor, Reactive distillation, Extractive fermentation, Membrane Reactors. **PI in Industrial Practice**: Methodology, Application, Contribution to sustainable development, Improvement in existing plant and process synthesis, De-bottle-necking, Integrated plants.	8
5	**PI for Plant Safety**: Traditional Approach, Strategies.	3

8. Books:

(A) Text Books

S. No.	Authors / Name of Book / Publisher	Year of Publication
1.	Stankiewicz, A., and Moulijn. J. A., Re-engineering the Chemical Processing Plant: Process Intensification, Marcel Dekker, Inc., New York.	2004

(B) Reference Books

S. No.	Authors / Name of Book / Publisher	Year of Publication
1	Mizrahi, J., Developing an Industrial Chemical Process: An Integrated Approach, CRC Press.	2002

1. Subject Code: 22CHT352 **Course Title: Multiphase Reactors**

2. Contact Hours: L:3 T:0 P:0

3. Credits: 3 Semester: VI

4. Pre-requisite: Nil.

5. Course Objective: To provide advance knowledge of various reactors used in chemical Industries and their working principles

6. Course Outcome:Upon completion of this course, the students will be able to:

i. Understand heterogeneous catalysis
ii. Understand the performance of various types of heterogeneous catalytic reactors
iii. Understand multiphase reactor hydrodynamics and contacting pattern
iv. Ability to design catalytic reactors

7. Details of Course:

Unit No.	Contents	Contact Hours
1.	**Introduction:** Reaction kinetics and ideal reactors. Fluid-solid reactions: catalytic and non-catalytic reactions.	4
2.	**Gas-Solid and Liquid-Solid Catalytic Reactions**: Effectiveness factor and Thiele modulus, Non-isothermal reactions, external mass transfer effects in two-phase and three-phase reactions, Selection of a ModelShrinking Core Model for Spherical Particles of Unchanging Size, Rate of Reaction for Shrinking Spherical Particles, Determination of the Rate-Controlling Step.	15
3.	**Gas-Liquid Reactors:**Fluid-Fluid Reactors: Design, Enhancement factor and Hatta number, various regimes of gas-absorption and reaction, Mass Transfer effect.	6
4.	**Introduction and Design of Multiphase Reactors**: Catalytic and non-catalytic reactors, Issues related to flow patterns and micro-, meso-reactor scale,performance/operating characteristics. Mechanically agitated reactors, bubble column/slurry bubble column reactors, fluidized bed, packed bed, trickle bed reactor and bioreactors. Novel reactors and process Intensification. Limitations of models used, applications of multiphase reactors for specific operation.	15

8. Books:

(A) Text Books

S. No.	Authors / Name of Book / Publisher	Year of Publication
1	Fogler, H. S., "Elements of Chemical Reaction Engineering," 5th Ed., Prentice-Hall of India, Delhi.	2016

(B) Reference Books

S. No.	Authors / Name of Book / Publisher	Year of Publication
1	Smith, J. M., "Chemical Engineering Kinetics," 3rd Ed., McGraw-Hill.	1981
2	Levenspiel, O., "Chemical Reaction Engineering," 3rd Ed., John Wiley.	2006

1. Subject Code: 22CHT402 Course Title: Molecular Modeling of Chemical Systems

2. Contact Hours: L:3 T:0 P:0

3. Credits: 3 Semester: VII

4. Pre-requisite: Nil.

5. Course Objective: The aim of course is to deal with the experimental and theoretical aspects of observations associated with numerous chemical engineering systems at molecular level.

6. Course Outcomes: Upon completion of this course, the students will be able to:

i. Understand the molecular basis of physical behavior in various Chemical Engineering systems.

ii. Develop the knowledge of methods, capabilities and limitations of molecular simulations.

iii. Decide whether the molecular simulation is an appropriate approach to solve concerned research problem.

7. Details of Course:

Unit No.	Contents	Contact Hours
1.	Fundamentals of molecular simulations: Ab-initio Methods, Basis Sets, HartreeFock Theory, Density Functional Theory, Geometry Optimization, VibrationalAnalysis.	8
2.	Classical statistical mechanics, elementary concepts of temperature, ensembles and fluctuations, partition function, ensemble averaging.	8
3.	Molecular Dynamics Methodology: Force Field, Integrating Algorithms, Periodic Box and Minimum Image Convention, Long Range Forces, Non Bonded Interaction.	8
4.	Temperature Control, Pressure Control, Estimation of Pure Component Properties, Radial Distribution Function; Molecular Dynamics Packages.	8
5.	Monte Carlo simulation: Monte Carlo integration, simple biasing methods, importance sampling, Markov chain, transition-probability matrix, detailed balance, Monte Carlo simulation in different ensembles, Monte Carlo simulation for polymer; Advanced applications.	8

8. Books:

(A) Text Books

S. No.	**Authors / Name of Book / Publisher**	**Year of Publication**
1	Daan Frenkel and Berend Smit, Understanding Molecular Simulation: From Algorithms to Applications,2nd Ed., Academic Press, New York.	2002
2	M.P. Allen and D.J. Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford	1987

1. Subject Code: 22CHT452 Course Title: Process Industry 4.0

2. Contact Hours: L:3 T:0 P:0

3. Credits: 3 Semester: VIII

4. Pre-requisite: Nil.

5. Course Objective:It is designed to deepen students knowledge in digitizing the industries using advanced technologies in process instrumentation and control, process modelling, industrial communication, human-computer interface, connectivity, machine learning, IoT (IoT), and industrial robotics.

6. Course Outcomes: Upon completion of this course, the students will be able to:

i. Understand the opportunities, challenges brought about by Industry 4.0 for benefits of organizations and individuals

ii. Analyze the effectiveness of Smart Factories, Smart cities, Smart products and Smart services

iii. Apply the Industrial 4.0 concepts in a manufacturing plant to improve productivity and profits

iv. Evaluate the effectiveness of Cloud Computing in a networked economy

7. Details of Course:

Unit No.	Contents	Contact Hours
1.	**History and Introduction:** Definition of Industry 4.0, Development of Digitization and the Networkeconomy, Comparison of Industry 4.0FactorandToday's factory,Mostimportant things that will change with Industry 4.0,Difference betweenconventional automation and Industry4.0, Internet of Things (IoT) & Industrial Internet of Things (IIoT) &Internet of Services, Big data, Cyber-Physical System (CPS),Customization of products, Digital Twins	8
2.	**Technologies for Enabling Industry 4.0:** Cloud Computing / Cloud Manufacturing, Security issues within Industry 4.0networks, Definition of Cyber-Physical Systems (CPS) and Cyber-PhysicalProduction Systems (CPPS), Core elements of CPS and CPPS, Control theoryand real-time requirements, Communication in cyber-physical systems, DesignMethods for Cyber-physical Systems, Applications for cyber-physical systems,Resource-based view of a firm, Data as a new resource for organizations,Harnessing and sharing knowledge in organizations, Cloud Computing Basics,Cloud Computing and Industry 4.0, ML, AI	8
3.	**Case studies based on type of chemical/process industries** a. Industry 1 Power plant b. Industry 2 Refineries c. Industry 3 Food and pharma	8
4.	**Safety and security in networked production environments** Safety in Industry 4.0, Safety for connected machines and systems,	8

	Safety inhuman-robot cooperation, Safety Optimization through Industry 4.0, Securityrisks in Industry 4.0 and AI, Approach to Cyber-Physical Security in Industry4.0, Standard for control systems, security of cloud, IEC62-443.	
5	**Future prospects of IIoT**	04

8. Books:

(A) Text Books

S. No.	**Authors / Name of Book / Publisher**	**Year of Publication**
1	Sudip Misra, Chandana Roy, Anandarup Mukherjee, Introduction to Industrial Internet of Things and Industry 4.0, 1st Ed., CRC Press.	2020
2	Denis Constales, et. al., Advanced Data Analysis & Modelling in Chemical Engineering, 1st Ed., Elsevier.	2016

(B) Reference Books

S. No.	**Authors / Name of Book / Publisher**	**Year of Publication**
1	Keith R. Holdaway, Harness Oil and Gas Big Data with Analytics: Optimize Exploration and Production with Data-Driven Models, 1st Ed., Wiley.	2014