THE INTERPLAY OF CHEMISTRY AND ENGINEERING : FOUNDATIONS

OBJECTIVES

→ Fundamental Concept of Chemistry and Their Relevance to Engineering

→ Bridge Course: Connection Basic Chem to Engg. Application

→ Innovations at the Intersection of Chemistry & Engineering

→ Basic Engg Chem. Course at VIT-AP

→ Lab course & Safety in Lab

WHO IS AN ENGINEER

→ Engineers → apply scientific principles to analyze, design, invent, code, build, and create to solve all sorts of problems and make the world a better place, One of their most important tools in their own creativity.

→ Engineers solve problems using maths, science, & technology.

WORLD PROBLEMS v/s ROLE OF ENGINEERS

PROBLEMS	Role of Engg:-	E.g. of Engg. Solutions
Climate Change	Develop sustainable tech, design carbon captur syst, create eco friendly materials.	Renewable energy (solar, wind) EVs, green buildings
War (conflict & security)	Innovate non lethal defence syst; enhance cybersecurity; improve safety & communication	Surveillance drones, cyber security frameworks, communication networks
Poverty	Design affordable techs; develop low cost housing and water purification, create jobs thru tech transfer	low-cost solar lighting, 3D-printed housing, inexpensive medical devices.
Energy crisis	Develop efficient energy/conversion techs; improve power grids; explore alternative fuels	High capacity Batteries, hydrogen fuel cell, smart energy systems.

CHEMISTRY – RELEVANCE TO ENGG:

↳ Fundamentally imp to all branches of engg. It provides the scientific basis for understanding materials, their properties, and how they interact, which is crucial for designing, developing and improving various technologies and processes.

Why the name Silicon Valley?

why are quantum computers expensive to maintain?

IMPORTANCE OF CHEMISTRY FOR CSE & IT

1. Chemistry's Role in Computer Sci.
   - Chem → crucial to CSE as it helps understanding how computers function at their most basic level.

2. Software Applications in Chemistry.
   - Numerous software tools are used in chem for Research & Analysis.

3. Computational Drug Discovery.
   - Computer-aided methods streamline drug dev.
   - Benefits include:
     → Reduced Costs
     → Increased success Rates
     → faster drug development process.

4. AI & ML in Drug Discovery
   - Revolutionize drug discovery by:
     → Accelerating identification of potential drug candidates.
     → optimizing clinical trials.
     → Personalizing treatments

5. Machine Learning Application
   - ML algos. analyze vast datasets to:
     → predict molecular properties
     → Identify promising compounds
     → optimize drug candidates

Importance of Chem. for ECE & EEE

- Help E&TC / Electrical students understand conductors, semiconductors, sensors and insulators.
- Engineers must know e⁻'s, conduction, magnetic nature.
- Electronic sensors & biosensors (detection, diagnosis) need chemistry for fabrication & design.
- In bio sensors, devices detect signals via chemical rxn.

Importance of Chem for Mech & Civil

- Machine / vehicle operation depends on fuel; chem needed to study efficiency, quality, properties
- Choosing fuels needs knowledge of exhaust effects.
- Lubricants reduce friction, selection needs chem knowledge
- Civil enggs analyze soil nature / props. before constructⁿ
- Manufacturing ceramics / refractories for specific purposes needs chem.

COURSE CODE : CHY 1009

COURSE TITLE : Chemistry & Environmental Studies.

STATES OF MATTER

Matter: → has mass & occupies space

Solid $\xrightarrow{\text{Melting}}$ Liquid $\xrightarrow{\text{Vaporization}}$ Gas $\xrightarrow{\text{Ionization}}$ Plasma

Solid $\xleftarrow{\text{freezing}}$ Liquid $\xleftarrow{\text{Condensation}}$ Gas $\xleftarrow{\text{Deionization}}$ Plasma

State	shape	Volume	Particle arrangement	examples
solid	fixed	fixed	Tightly packed	Ice, wood, metal
liquid	variable	Fixed	close, less ordered	water, oil, alcohol
Gas	Variable	variable	Far apart, random	Air, CO_2, helium
Plasma	Variable	Variable	Ionized, charged	Lightning, stars

- Bose-Einstein Condensate → 5th state of matter

Adsorption isotherm

Sorption: one substance taking up another

Adsorption: Surface phenomena - molecules (adsorbate) called on the surface of another (adsorbent)

Adsorbate: Substance being Adsorbed

Adsorbent: substance Adsorbing the adsorbate

• Increase adsorbate concⁿ on the surface

Example: • Gas molecule adhering to solid surface
• Water vapour condensing on cold surface
• pollutant removal from water/air using activated Carbon

Absorption: One substance (absorbate) penetrate into the bulk of another surface (absorbent).
└ volume phenomenon, not just surface phenomenon

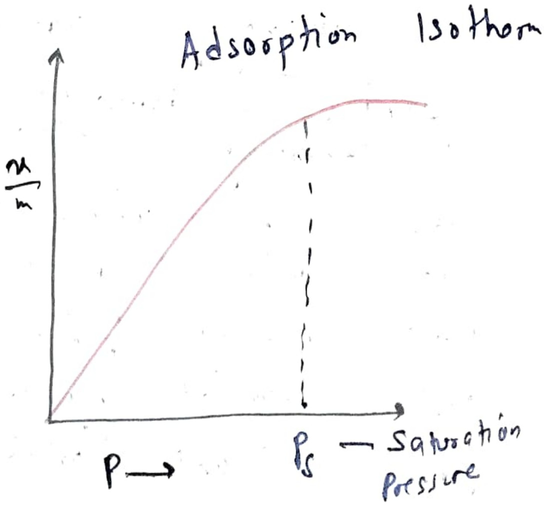
Examples: • sponge soaking water
• CO_2 dissolving in liq.
• Sponge absorbing spilled water/liquid

• Sorption: → process where one substance (sorbate) is taken up by another (sorbent)

Adsorption Isotherms - Graph & Applications

↓ graph showing variation in amount adsorbed (x/m) v/s pressure (P) at const temp.

• Types:
1. Langmuir Isotherm
2. Freundlich Isotherm
3. BET theory



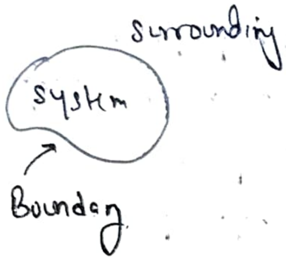
Applications

• Removing water & air pollutants
• sensors development
• drug delivery ctrl
• catalytic Converters design

THERMODYNAMICS

focus on r/n b/w heat, work and internal energy, & the laws that govern these transformation

L branch of physical science that deals with the study of energy, in various forms and how it is stored and transformed within a system.



* Thermodynamic System

✓ quantity of matter or a region of space chosen to study

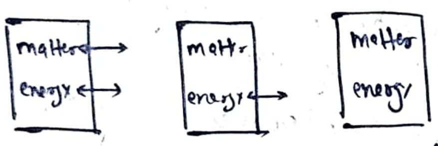
* Boundary

✓ A real or imaginary layer that separates the system from its surroundings

* Surrounding

✓ physical space outside the system boundary

Types of system



open system | closed sys | isolated system

Thermodynamic variables → physical properties used to describe the state of thermodynamic system

- Intensive
  - Independent of amt of substance.
  - Temp(T), Pressure(P), Density(ρ), Chem potential (μ)
- extensive
  - depend on amt of substance.
  - Vol^n(V), Internal Energy(U), Entropy(S), No. of particles (n), Enthalpy (H)

$$\frac{\text{* Extensive}}{\text{Extensive}} = \text{Intensive}$$

$$\left[\frac{\text{mass}}{\text{vol}^n} = \text{density}\right]$$

Thermodynamic Processes & Paths

↳ Physical change in a system that alters its thermodynamic state (characterized by variables like pressure, temp, volᵐ, etc)

→ Some special processes

- Isobaric process – const. pressure process
- Isothermal process – const. temp process
- adiabatic process – const. heat (no heat exchange) $Q=0$
- isochoric process – const volᵐ process
- isoentropic process – const. entropy process

LAWS OF THERMODYNAMICS

↳ fundamental principles that describe how energy moves and changes in physical systems particularly involving heat, work & internal energy.

* Zeroth Law of Thermodynamics

- statement: If sys. A is in thermal eqbᵐ with sys B. and sys B is in thermal eqbᵐ with sys C. then A & C are also in thermal eqbᵐ

Implication:
↓
- Defines temp as a measurable property.
- Basis for using thermometers

* First Law of Thermodynamics

- statement: Energy can neither be created nor destroyed, only transformed from one form to another.

- Implications
- Total energy → conserved
- Heat & work are diff form of energy transfer

$\boxed{\Delta U = Q - W}$

$\Delta U \equiv$ change in internal energy
$Q =$ Heat added to sys
$W =$ Work done by sys

Example: In a steam engine → Heat supplied ⇒ increases int. energy + does work by expanding steam

$\boxed{Q = \Delta U + Q}$

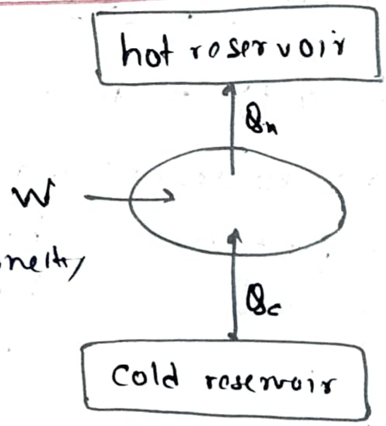
Real world applications:
– Power plant – any system converting heat to work
– Car engines

* Second Law of Thermodynamics – Entropy law

→ Kelvin Plank Statement : No heat engine can operate in a cycle and convert all heat absorbed from a heat source into work
e.g. Engine

→ Clausius Statement : Heat cannot spontaneously flow from a colder body to a hotter body w/o ext. work.
e.g. refrigirator

→ Entropy Statement : In any spontaneous process, the total entropy of the universe increases ∴ $\boxed{\Delta S_{universe} > 0}$



• Implications →
→ Explains the irreversibility of natural process
→ sets a dirⁿ : from order to disorder
→ Basis for heat engines, refrigerator, & spontaneity

* Third Law of Thermodynamics

→ statement : As the temp of a sys approaches absolute zero ($T \to 0$), the entropy of a perfect crystal approaches zero.

$S \to 0$ & $T \to 0$

→ Implications :
→ impossible to reach absolute zero in a finite number of steps
→ reference point for absolute entropy

? How are these law & Thermodynamic principles used in air coolers, air conditioners, refrigerators, heat pumps, heat engines, and IC engine system?

Kinetics & Catalysis

Chemical kinetics
study of rxn rates and factors affecting them.
catalysis : Acceleration of chem. rxn by catalysts

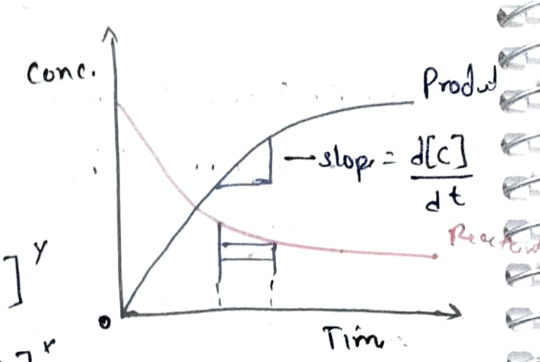
rxn rate – speed at which reactants are converted to products, measured by how fast reactants are consumed or products are formed

Factors Affecting Rate : → conc. of reactant
→ temp. of rxn
→ Presence of catalyst
→ surface area of solid/liq reactants or catalysts

General Reaction

$$aA + bB \rightarrow cC + dD$$

a, b, c, d → stoichiometric coeff.



Rate Equation :

$$\text{Rate} \propto [A]^x [B]^y$$

$$\text{Rate} = k[A]^x [B]^y$$

Rate law : Expression that show that rate depends on concⁿ of reactants.

$\text{Rate} \propto [A]^x [B]^y \Rightarrow \text{Rate} = k[A]^x [B]^y$

$x + y$ = order of rxn

→ zero order: no change in rate when conc. changed.
→ first order: Change in conc. gives proportional changes in rate
→ second order: change in concentration changes rate by the square of the concentration change. such as 2^2 or 3^2, etc

→ rate const. does not depend on concⁿ

What is Effect of temp on the rate? kinetics of ozone layer depletion.

Catalyst : A substance that alters the rate of rxn w/o being permanently consumed.

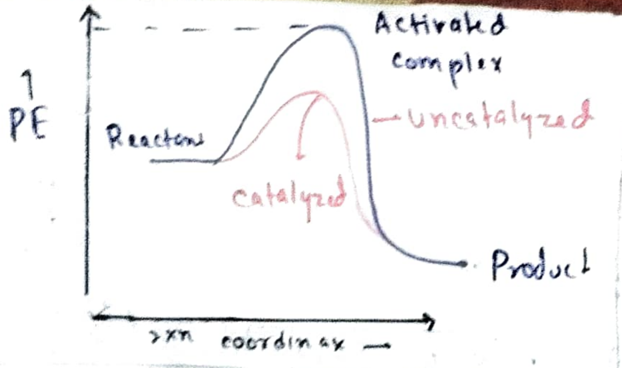
How catalyst work :
- Provide an alternative rxn pathway with lower E_a
- lower energy barrier → rxn occur faster

Types of Catalysts

1. Homogenous Catalysis – Catalyst & rxn in same phase
2. Heterogeneous Catalysis – catalyst & reactant → diff phase

Applicaⁿ
- Fischer – Tropsch synthesis
- Haber – Bosch process
- 3 way automotive catalyst

Other types → Homogeneous
Heterogeneous
Biological catalysis (enzyme)



ELECTROCHEMISTRY & CHEMICAL SENSORS

→ Study the relation b/w Electricity and chemical reactions ~~relation~~

Practical Applications:

1. Electrochemical industries
2. Biomedical application
3. Energy conversion & storage
4. Fuel cells
5. Corrosion engineering
6. Environmental remedies

Technologies based on Electrochem.

- Energy storage
- Sensing
- Corrosion prevention
- Organic electrosynthesis
- Industrial electrolysis
- Energy conversion

- Electrode potential – Tendency of an electrode to gain/lose e^- when in contact with its ion soln.
- Electrode :- Electrical conductor allowing e^- transfer ~~from~~ to/from a chem. syst.
- Half-Cell – Single electrode in a soln of its ions.
- Oxidn/Redn – Pot. diff. due to metal loosing e^- (oxidn) or gaining e^- (redn)
- Standard Electrode Potential (E°) – Measured under std. condn 298 K, 1 atm, 1 M ion concn.
  - Reference: SHE (standard Hydrogen electrode), $E^\circ = 0$ V
- Electrochemical cells :- Two half cells with diff pot. connected galvanic (voltaic) cell.
  - spontaneous redox rxn generates electrical energy.
  - Formula: $\boxed{E_{cell} = E_{cathode} - E_{anode}}$