
The Interplay of Chemistry and Engineering: Foundations
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Objectives

- ❖ Fundamental Concepts of Chemistry and Their Relevance to Engineering
- ❖ Bridge Course: Connecting Basic Chemistry to Engineering Applications
- ❖ Innovations at the Intersection of Chemistry and Engineering
- ❖ Basic Engineering Chemistry Course at VIT-AP
- ❖ Lab Course and 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 is their **own creativity**.
- Engineers solve problems using math, **science**, and technology.

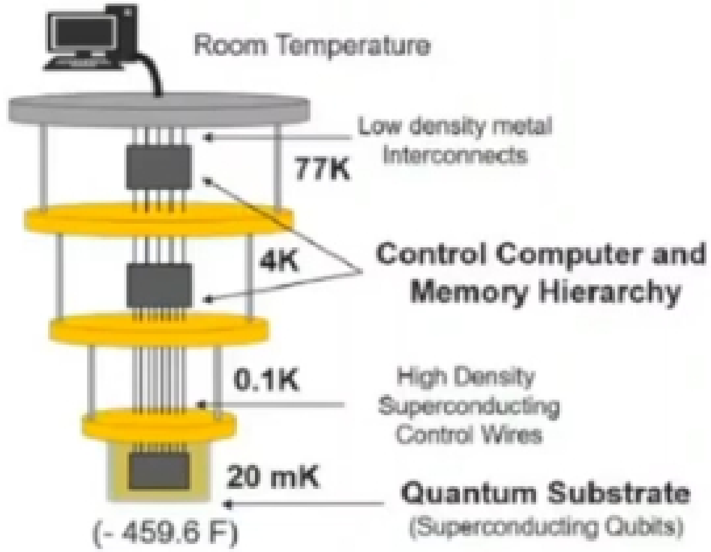
World Problems vs. Role of Engineers

Problem	Role of Engineers	Examples of Engineering Solutions
Climate Change	Develop sustainable technologies; design carbon capture systems; create eco-friendly materials.	Renewable energy (solar, wind), electric vehicles, green buildings.
War (Conflict & Security)	Innovate non-lethal defense systems; enhance cybersecurity; improve safety and communication.	Surveillance drones, cybersecurity frameworks, communication networks.
Poverty	Design affordable technologies; develop low-cost housing and water purification; create jobs through tech transfer.	Low-cost solar lighting, 3D-printed housing, inexpensive medical devices.
Energy Crisis	Develop efficient energy storage/conversion technologies; improve power grids; explore alternative fuels.	High-capacity batteries, hydrogen fuel cells, smart energy systems.

Chemistry- Relevance to Engineering

- Chemistry is fundamentally important to all branches of engineering. 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.

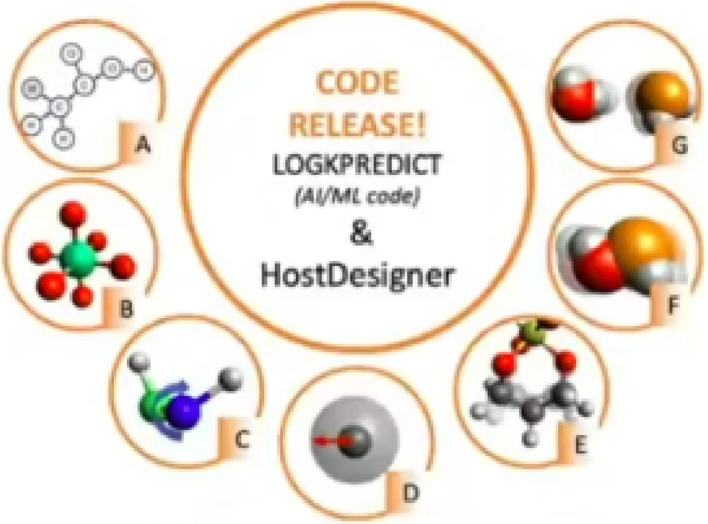
Why the name Silicon Valley?

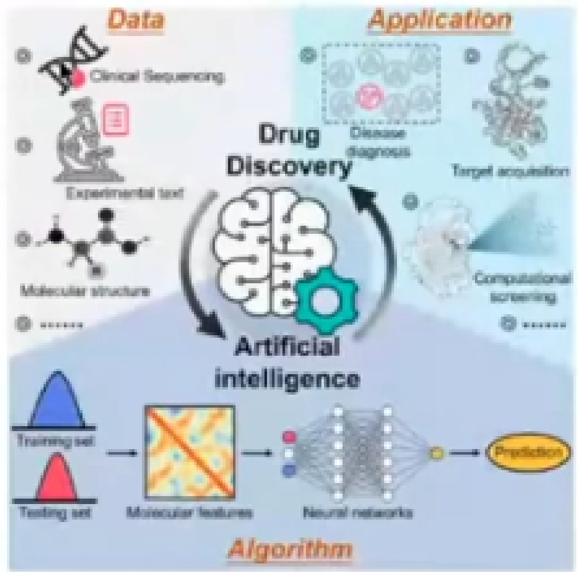


Why are quantum computers expensive to maintain?

Importance of Chemistry for CSE & IT

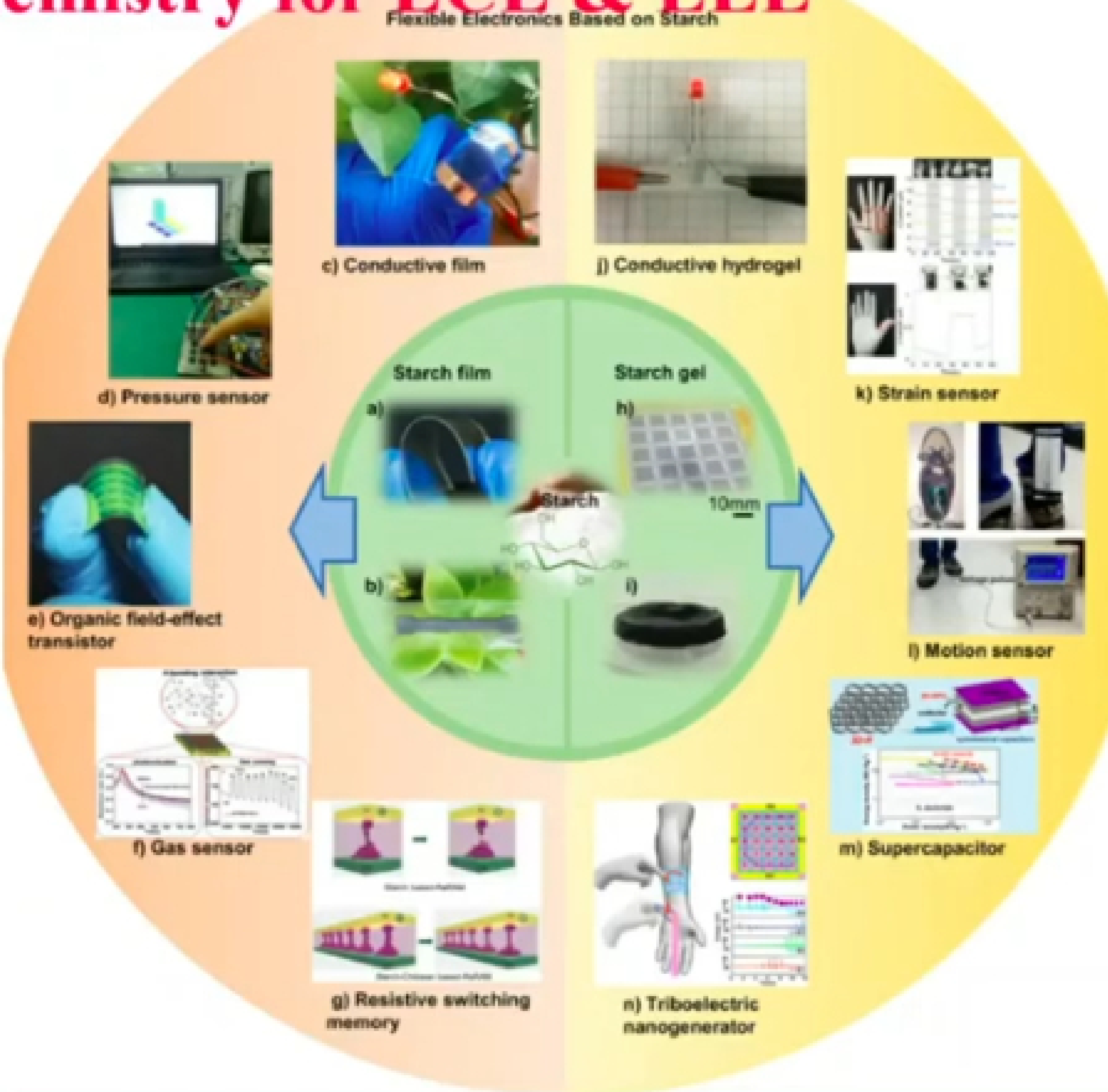
- ❖ Chemistry is crucial to computer science because it enables us to comprehend how computers function at their most basic level.
- ❖ Numerous software applications are employed in the field of chemistry for research and analysis.
- ❖ Computational drug discovery, utilizing computer-aided methods, is crucial for streamlining the drug development process, reducing costs, and increasing success rates.
- ❖ AI and ML are revolutionizing drug discovery by accelerating the identification of potential drug candidates, optimizing clinical trials, and personalizing treatments.
- ❖ Machine learning (ML) algorithms can analyze vast datasets to predict molecular properties, identify promising compounds, and optimize drug candidates.





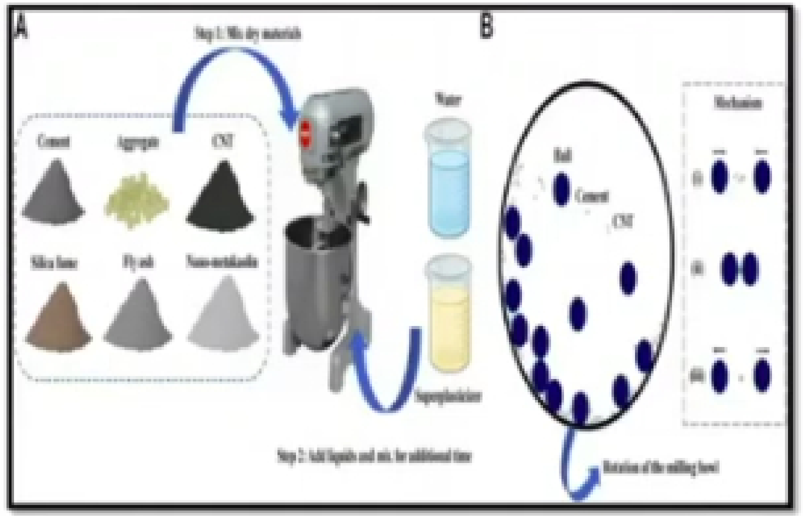
Importance of Chemistry for ECE & EEE

- ✓ Engineering chemistry aids E&TC and Electrical students in understanding conductors, semiconductors, sensors, and insulators.
- ✓ An Electronic or Electrical engineer must know about electrons, conduction, magnetic nature, etc.
- ✓ Electronic sensors and biosensors, vital for detection and diagnosis, require knowledge of chemistry for fabrication and design.
- ✓ Chemistry plays a crucial role in biosensors, where an electronic device receives signals only through chemical reactions.



Importance of Chemistry for Mechanical & Civil

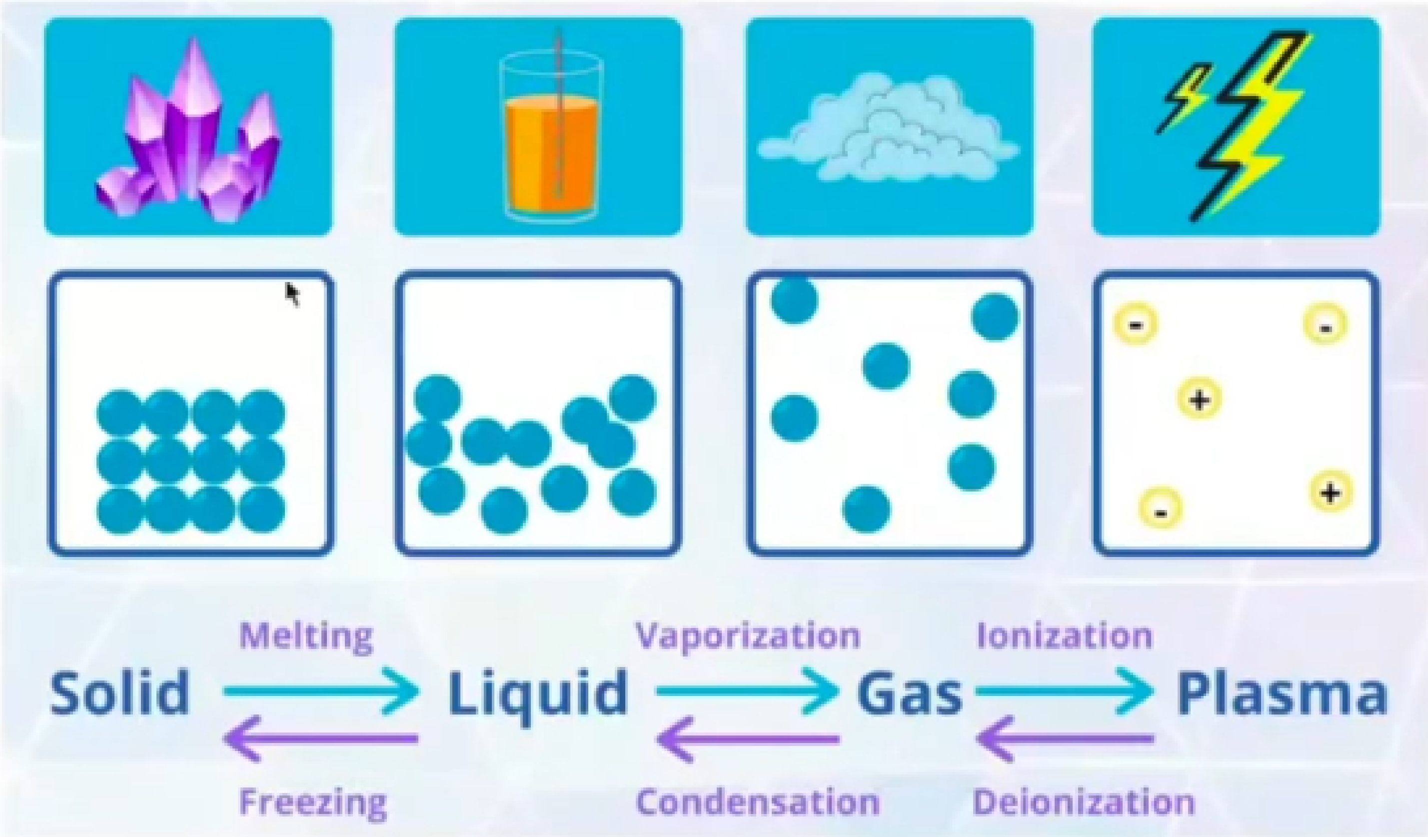
- The operation of any machine or vehicle relies on fuel, and studying the efficiency, quality, and properties of fuel is only possible through the lens of chemistry
- The selection of a suitable fuel by a mechanical engineer requires consideration of its exhausts, where knowledge of chemistry proves invaluable.
- Lubricants, essential for reducing friction between metal surfaces, require a mechanical engineer to possess knowledge of suitable lubricants for specific environments.
- Selecting a location or area for construction requires a civil engineer to analyze the nature and properties of the soil.
- To meet the manufacturing requirements of specific ceramics or refractories for suitable purposes, one must possess knowledge of chemistry.




Course Code: CHY1009
Course Title: Chemistry and Environmental Studies
QUANTUM COMPUTING
FOR BETTER CATALYSTS
FOR GREEN HYDROGEN

States of Matter

- **Matter** is anything that has Mass and takes up space



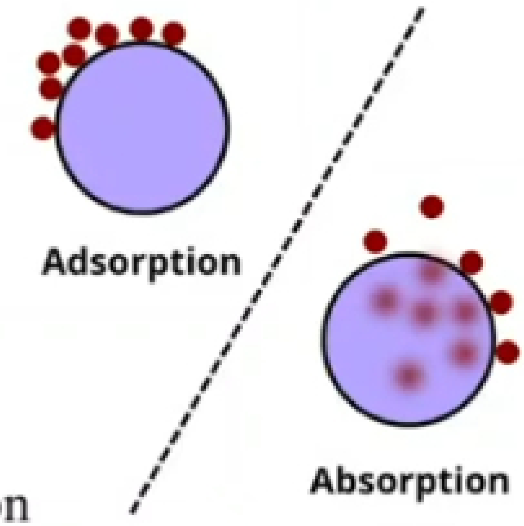
States of Matter

State	Shape	Volume	Particle Arrangement	Examples
Solid	Fixed	Fixed	Tightly packed, ordered	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 as a fifth state of matter**

Adsorption isotherms

- Sorption, adsorption, and absorption are terms related to how substances interact with each other, particularly when one substance is taken up by another.
- **Adsorption**: is a surface phenomenon where molecules of a substance (the adsorbate) accumulate on the surface of another substance (the adsorbent).
- It's a process that increases the concentration of the adsorbate on the surface.
- **Adsorbate:** The substance being adsorbed
- **Adsorbent:** The substance that adsorbs the adsorbate



Examples:-

1. Gas molecules adhering to the surface of a solid material
2. Water vapor condensing on a cold surface
3. The removal of pollutants from water or air using activated carbon

Adsorption isotherms

- **Absorption**: is a process where one substance (the absorbate) penetrates into the bulk of another substance (the absorbent)
- It's a volume phenomenon, not just a surface phenomenon

Examples:-

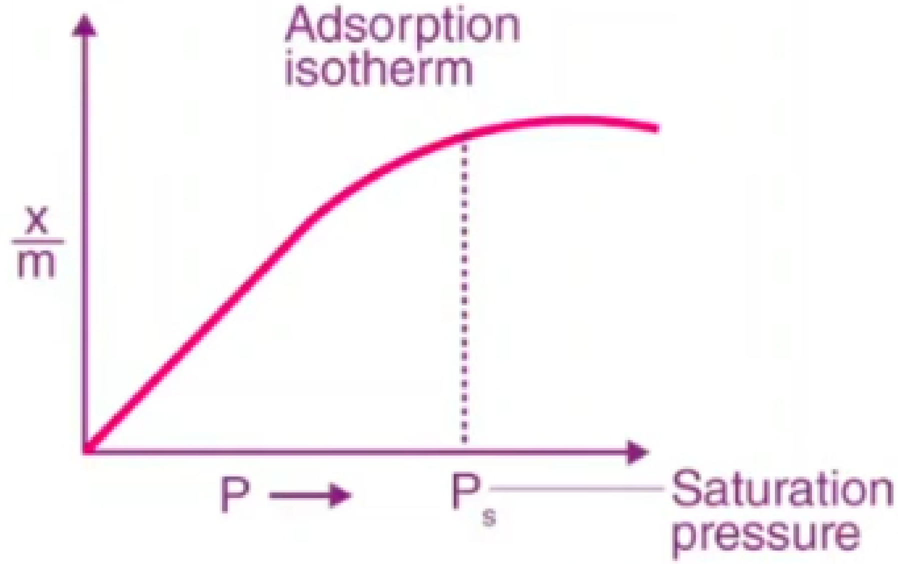
1) A sponge soaking up water.
2) Carbon dioxide dissolving in a liquid
3) A sponge absorbing spilled liquid

Sorption is a broad term that refers to the process where one substance (the sorbate) is taken up by another (the sorbent).

Adsorption isotherms

➢ An adsorption isotherm is a graph that represents the variation in the amount of adsorbate(x) adsorbed on the surface of the adsorbent with the change in pressure at a constant temperature.

➢ Different adsorption isotherms have been proposed by different scientists, namely,

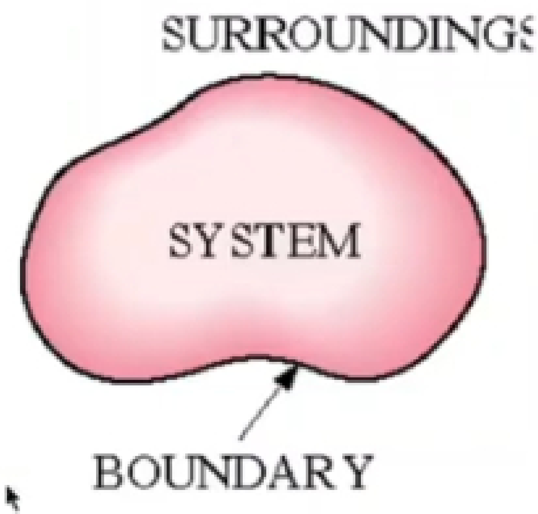


- **Langmuir isotherm**
- **Freundlich isotherm**
- **BET theory**
- Some important applications include **removing pollutants from water and air, developing sensors, controlling drug delivery, and designing catalytic converters**

Thermodynamics

❖ **What is thermodynamics?**

Thermodynamics is the branch of physical science that deals with the study of energy, its various forms, and how it is stored and transformed within **a system**. It primarily focuses on the relationships between heat, work, and internal energy, and the laws that govern these transformations.



❖ **Thermodynamic System**

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

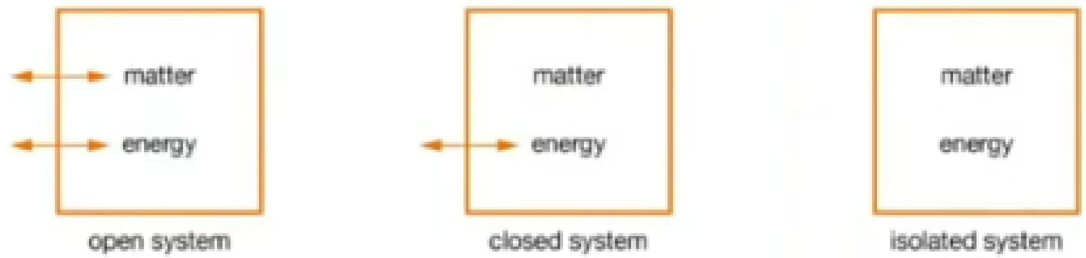
❖ **Boundary**

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

❖ **Surroundings**

✓ physical space outside the system boundary

❖ **Types of Systems**



Thermodynamics

❖ Thermodynamic Variables

- **Thermodynamic variables** are physical properties used to describe the state of a thermodynamic system. They are classified into two main categories: **intensive** and **extensive** variables.

❖ Types of Thermodynamic Variables

- **A. Intensive Variables**
- Independent of the amount of substance.
- Examples: Temperature (T), Pressure (P), Density (ρ), Chemical potential (μ)
- **B. Extensive Variables**
- Depend on the amount of substance.
- Examples: Volume (V), Internal energy (U), Entropy (S), Number of particles (n), Enthalpy (H)

✓ The ratio of two extensive variables can result in an intensive variable.

- For example, density = mass/volume.

Thermodynamics

❖ Thermodynamic Processes & Paths

- A **thermodynamic process** is any physical change in a system that alters its thermodynamic state (characterized by variables like pressure, temperature, volume, etc.).

✓ **some special processes:**

- ❑ isobaric process - constant pressure process
- ❑ isothermal process - constant temperature process
- ❑ adiabatic process - no heat is exchanged: $Q=0$
- ❑ isochoric process - constant volume process
- ❑ isentropic process - constant entropy process

Thermodynamics

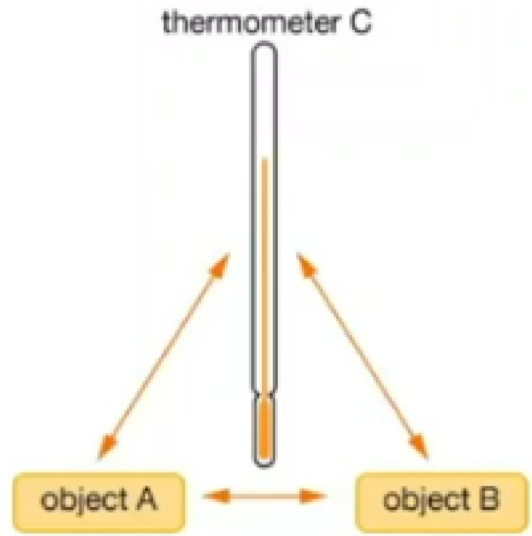
➢ The **Laws of Thermodynamics** are fundamental principles that describe how energy moves and changes in physical systems, particularly involving **heat**, **work**, and **internal energy**.

❖ **Zeroth Law of Thermodynamics**

- **Statement**: If system A is in thermal equilibrium with system B, and system B is in thermal equilibrium with system C, then A and C are also in thermal equilibrium.

Implication:

- Defines **temperature** as a measurable property.
- Basis for using **thermometers**.



Thermodynamics

❖ First Law of Thermodynamics – *Law of Energy Conservation*

- Statement:
  Energy cannot be created or destroyed, only transformed from one form to another.
- $$\Delta U = Q - W,$$
- Where: ΔU = change in internal energy, Q = heat added to the system, W = work done by the system.
- **Implication**:

✓ Total energy is conserved.

✓ Heat and work are **different forms of energy transfer**.

✓ Heat is supplied to water to produce steam that pushes a piston. (**in Steam Engine or Heat Engine**)- Heat input → internal energy increase + work done by expanding steam- $Q = \Delta U + W$

✓ **Real-world**: All power plants and car engines operate on this principle.

Thermodynamics

❖ **Second Law of Thermodynamics** – *Entropy Law*

➢ **Kelvin-Planck 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 without external work.

e.g. refrigerator

➢ **Entropy Statement:** In any spontaneous process, the total entropy of the universe increases:

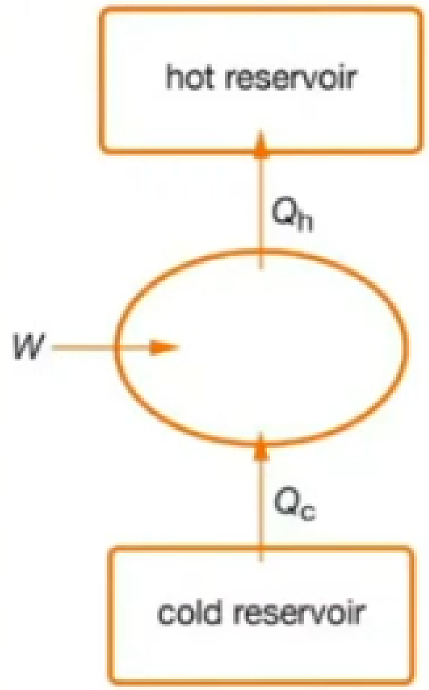
$$\Delta S_{universe} > 0$$

- **Implication**:

✓ Explains the **irreversibility** of natural processes.

✓ Sets a direction: **from order to disorder**.

✓ Basis for heat engines, refrigerators, and spontaneity



Thermodynamics

❖ Third Law of Thermodynamics

Statement: As the temperature of a system approaches absolute zero ($T \rightarrow 0$), the entropy of a perfect crystal approaches zero.

$$S \rightarrow 0 \text{ as } T \rightarrow 0$$

Implication:

✓It's impossible to reach **absolute zero** in a finite number of steps.

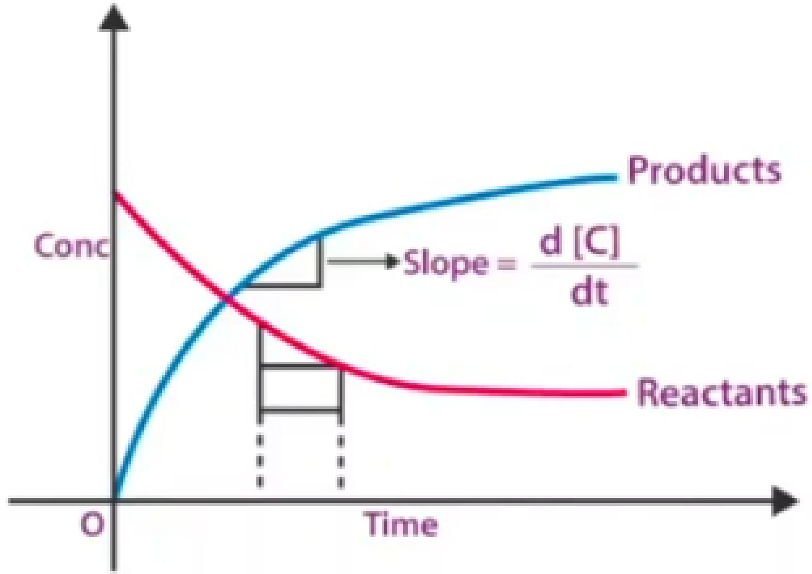
✓Provides a reference point for **absolute entropy**.

✓How are these Laws and Thermodynamic principles used in air coolers, air conditioners, refrigerators, heat pumps, heat engines, and IC engine systems **?**

Kinetics and Catalysis

- ❖ Chemical kinetics is the study of reaction rates and how they are affected by various factors, while catalysis involves the acceleration of chemical reactions by substances called catalysts

Reaction Rate:- The speed at which reactants are converted into products, typically measured by how fast reactants are consumed or products are formed.



- ❖ Rates of reactions affected by four factors

1. concentrations of reactants
2. temperature at which the reaction occurs
3. presence of a catalyst
4. surface area of solid or liquid reactants and/or catalysts

- ❖ For a reaction given by:

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

- where a, b, c, and d are the stoichiometric coefficients of the reactants or products, the rate equation for the reaction is given by:
- **Rate $\propto [A]^x[B]^y \Rightarrow$ Rate $= k[A]^x[B]^y$**

Kinetics and Catalysis

- ❖ **Rate law** – expression that shows that rate depends on concentrations of reactants
- ❖ **Rate $\propto [A]^x[B]^y \Rightarrow$ Rate $= k[A]^x[B]^y$**
- ❖ **X+ Y is the order of reaction**

✓ **zero order** – no change in rate when concentration changed

✓ **first order** – change in concentration 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 constant does not depend on concentration

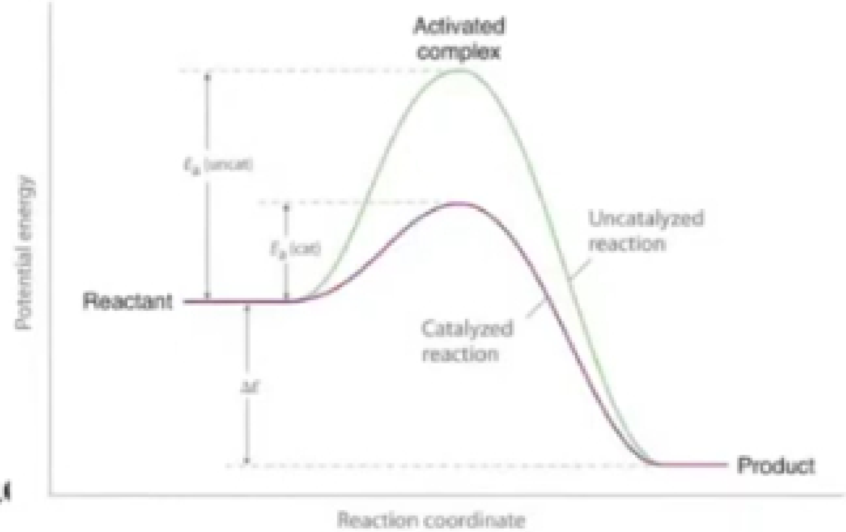
What is the Effect of temperature on the rate? Kinetics of ozone layer depletion

Kinetics and Catalysis

➢**Catalyst:** A substance that alters the rate of a reaction without being permanently consumed

❑**How Catalysts Work:**

They provide an alternative reaction pathway with a lower activation energy, effectively lowering the energy barrier for the reaction to occur



➢ **Types of Catalysis:**

Homogeneous Catalysis: Catalyst and reactants are in the same phase

Heterogeneous Catalysis: Catalyst and reactants are in different phases (e.g., solid catalyst in a liquid rea

Types of catalysis - Homogeneous, heterogeneous and biological catalysis. Applications: Fischer Tropsch synthesis, Haber-Bosch process and Three-way automotive catalysts.

Electrochemistry and Chemical Sensors

❖Electrochemistry studies the relationship between *electricity and chemical reactions*

❑ **Electrochemistry has several practical applications**

✓Electrochemical industries (for example, Chloralkaline industry)

✓Biomedical applications (electrodialysis, biosensors)

✓Energy conversion and storage systems

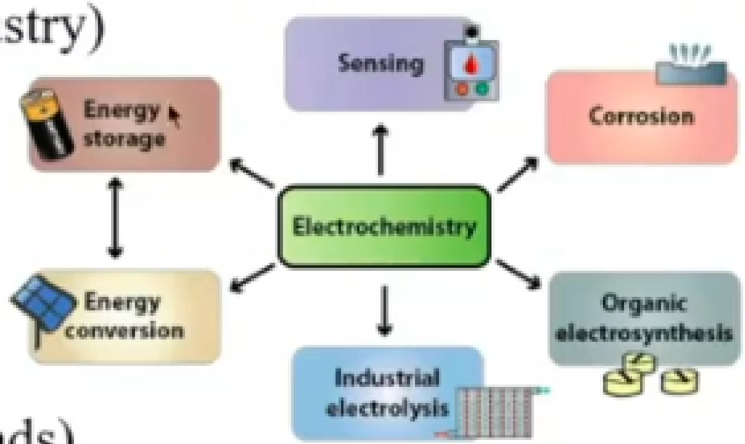
(Batteries, photovoltaics, and supercapacitors)

✓Fuel cells (Storing and utilization of energy in chemical bonds)

✓Corrosion engineering

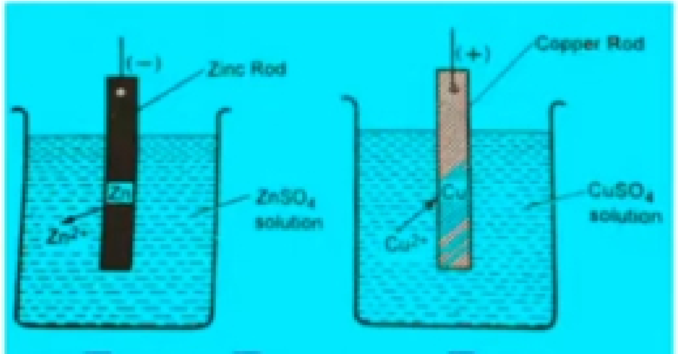
✓Environmental remedies (oxidative treatment of harmful dyes)

Some technologies based on Electrochemistry



Electrochemistry and Chemical Sensors

- **Electrode potential** is a measure of the tendency of an electrode to gain or lose electrons when it's in contact with a solution of its ions.
- **Electrode:** An electrical conductor that allows electrons to enter or leave a chemical system
- **Half-cell:** A single electrode immersed in a solution of its ions.
- **Oxidation or Reduction:** This potential difference arises because of the tendency of the metal to either lose electrons (oxidation) or gain electrons (reduction).



$$E_{cell} = E_{cathode} - E_{anode}$$

- **Standard Electrode Potential (E°):** The electrode potential is measured under standard conditions (usually 298 K, 1 atm pressure, and 1 M concentration of ions). The standard hydrogen electrode (SHE) is used as a reference and has a standard electrode potential of 0 V.
- **Electrochemical Cells:** By connecting two half-cells with different electrode potentials, a galvanic (or voltaic) cell is formed, and a spontaneous redox reaction can generate electrical energy

Electrochemistry and Chemical Sensors

- The **Nernst Equation** enables the determination of cell potential under non-standard conditions. It relates the measured cell potential to the reaction quotient and allows the accurate determination of equilibrium constants (including solubility constants)

$$\boxed{\Delta G = \Delta G^o + RT \ln Q}$$

At equilibrium Q = K

$\Delta G = -nFE_{cell}$ and $\Delta G^o = -nFE^o_{cell}$

Hence

Electrical potential energy

$$E_{cell} = E^o_{cell} - \frac{RT}{nF} \ln Q$$

$$E_{cell} = E^o_{cell} - \frac{0.0257}{n} \ln Q$$

Nernst equation

$$\boxed{E_{cell} = E^o_{cell} - \frac{0.0592}{n} \log_{10} Q}$$

Types of electrochemical cells, batteries, and fuel cells. Theories of corrosion, Anodic and cathodic protection, protective coatings, and corrosion inhibitors. Electroplating, electro-machining, electro-winning, electro-refining, green electro-organic synthesis.