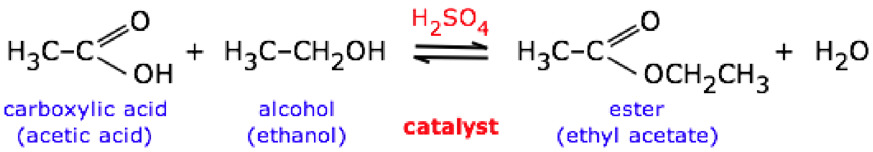
5.C) WHAT ARE CATALYSTS?

- Catalysts are substances that speed up a reaction but which are not consumed by it and do not appear in the net reaction equation.
- Catalysts have no effect on the equilibrium constant and thus on the equilibrium composition.
- Also — and this is very important — *catalysts affect the forward and reverse rates equally*; this means that catalysts have no effect on the equilibrium constant and thus on the composition of the equilibrium state. Thus a catalyst (in this case, sulfuric acid) can be used to speed up a reversible reaction such as ester formation or its reverse, ester hydrolysis:



- Catalysts function by allowing the reaction to take place through an alternative mechanism that requires a smaller activation energy. This change is brought about by a specific interaction between the catalyst and the reaction components. The rate constant of a reaction is an exponential function of the activation energy, so even a modest reduction of Ea Ea can yield an impressive increase in the rate.
- Catalysts provide alternative reaction pathways

Types of Catalytic Reaction

Catalysts are conventionally divided into two categories: *homogeneous* and *heterogeneous*. *Enzymes*, natural biological catalysts, are often included in the former group, but because they share some properties of both but exhibit some very special properties of their own, we will treat them here as a third category.

1. **Homogenous Catalysis**

   In this type of catalysis reaction, both catalyst and reactant remain in the same phase. Here, the catalyst either remains uniformly dispersed in the gas phase or gets dissolved in the reactant. So, the number of collisions between reactant and catalyst is maximum. These catalysts are used in various industrial applications. They allow for an increase in reaction rate without an increase in temperature.

   Catalyst examples:
   - **Sulfuric acid (H_2SO_4)** – used in esterification and hydration reactions
   - **Hydrochloric acid (HCl)** – used in hydrolysis
   - **Nitric oxide (NO)** – used in the oxidation of sulfur dioxide in the lead chamber process
   - **Aluminium chloride ($AlCl_3$)** – used in Friedel-Crafts alkylation
   - **Phosphoric acid (H_3PO_4)** – used in hydration of alkenes

2. **Heterogeneous Catalysis**

   Unlike homogenous catalysis, the catalyst exists in a different phase than the reactant in this type of catalysis reaction. Generally, the catalyst remains solid, while the reactants are gaseous or liquid. The catalyst does not dissolve into the reacting mixture.

Instead, the catalytic action occurs by adsorption, where catalyst acts as adsorbent and reactant acts as adsorbate.

Catalyst examples:

- **Iron (Fe)** – used in the Haber process (NH_3 synthesis)
- **Vanadium(V) oxide (V_2O_5)** – used in the Contact process (H_2SO_4 production)
- **Nickel (Ni)** – used in hydrogenation of alkenes
- **Platinum (Pt)** – used in catalytic converters and hydrogenation
- **Palladium (Pd)** – used in coupling reactions and hydrogenation

3. **Biocatalysts** – Enzymes that speed up biological reactions

Catalyst examples (enzymes):

- **Amylase** – breaks down starch into sugars
- **Lipase** – catalyzes hydrolysis of lipids
- **Protease** – breaks down proteins into amino acids
- **Lactase** – breaks lactose into glucose and galactose
- **DNA polymerase** – catalyzes DNA synthesis
- **Catalase** – decomposes hydrogen peroxide into water and oxygen

Role of Reaction Conditions

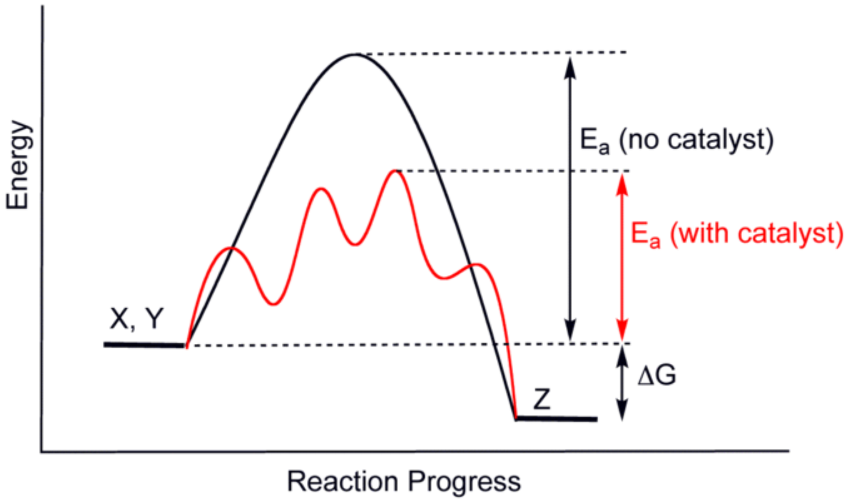
Reaction conditions significantly affect reaction rates and yields. Key factors include:

1. **Temperature** – Increasing temperature generally increases reaction rates by providing more kinetic energy to reactant molecules, overcoming activation energy barriers.
2. **Pressure** – In gas-phase reactions, higher pressure favours reactions that produce fewer gas molecules (Le Chatelier’s Principle).
3. **Concentration** – Higher reactant concentration increases the frequency of collisions, leading to a higher reaction rate.
4. **Surface Area** – In heterogeneous catalysis, increasing the surface area of a solid catalyst improves its effectiveness.
5. **Solvent Effects** – The choice of solvent can influence reaction pathways, solubility of reactants, and stabilization of transition states.
6. **pH** – Important in acid-base catalysis and enzyme-catalyzed reactions where the activity depends on pH levels.

Together, catalysts and reaction conditions optimize chemical reactions for efficiency, selectivity, and economic viability, making them essential in industrial and biological processes.

Mechanism of Action of Catalysts

- Catalysts speed up chemical reactions by providing an alternative reaction pathway with a **lower activation energy**. While they do not alter the reaction’s thermodynamics (enthalpy change, ΔH), they facilitate the formation of products faster.



- The mechanism of action of a catalyst depends on whether it is homogeneous, heterogeneous, or a biocatalyst (enzyme).

1. Homogeneous Catalysis Mechanism

(Catalyst and reactants are in the same phase, usually liquid or gas)

- The catalyst forms an intermediate complex with the reactants, lowering activation energy.
- This intermediate then decomposes, releasing the product and regenerating the catalyst.
- Example: Acid-Catalyzed Esterification (Fischer Esterification)

$$\text{R-COOH} + \text{R'-OH} \xrightarrow{H^+} \text{R-COOR'} + H_2O$$

The acid (H^+) protonates the carboxyl group, increasing its electrophilicity. This facilitates nucleophilic attack by alcohol, leading to ester formation. The catalyst (H^+) is regenerated at the end.

2. Heterogeneous Catalysis Mechanism

(Catalyst is in a different phase, usually solid, while reactants are gases or liquids)

- The reaction occurs on the catalyst's surface, often through adsorption, reaction, and desorption.
- The catalyst provides active sites where reactant molecules bind and react more easily.
- Example: Hydrogenation of Ethene (Ni/Pt Catalyst)

$$C_2H_4 + H_2 \xrightarrow{\text{Ni/Pt}} C_2H_6$$

1. **Adsorption** – Ethene and hydrogen molecules attach to the metal surface.
2. **Activation** – Bonds within reactant molecules weaken.
3. **Reaction** – Hydrogen atoms add to the ethene, forming ethane.
4. **Desorption** – The product leaves the catalyst surface, regenerating the catalyst.

3. Enzyme Catalysis Mechanism (Biocatalysis)

(Catalyst is a biological enzyme, typically a protein, that speeds up reactions in living systems)

- Enzymes operate on the lock-and-key or induced-fit model, where the substrate binds to the enzyme's active site**.**
- They stabilize the transition state and lower activation energy.

Example: Breakdown of Hydrogen Peroxide by Catalase

$$2H_2O_2 \xrightarrow{\text{catalase}} 2H_2O + O_2$$

1. **Substrate binding** – Hydrogen peroxide binds to the catalase enzyme.
2. **Catalysis** – The enzyme facilitates bond-breaking and oxygen release.
3. **Product release** – Water and oxygen leave, and the enzyme is free to catalyze another reaction.