Lecture 6 “Fundamentals of homogeneous and heterogeneous catalysis: principles and applications”

Goal of the lecture: To study the fundamental principles of catalysis, distinguish between homogeneous and heterogeneous catalytic systems, understand the mechanisms of catalytic action, and explore their industrial and environmental applications.

Brief lecture notes

1. Definition and Basic Concept

Catalysis is the process by which the rate of a chemical reaction is increased by a substance called a **catalyst**, which participates in the reaction but is regenerated at the end of the process. Catalysts lower the **activation energy (E_a)**, allowing reactions to proceed faster or at lower temperatures.

The catalytic effect is shown schematically by the energy diagram below:

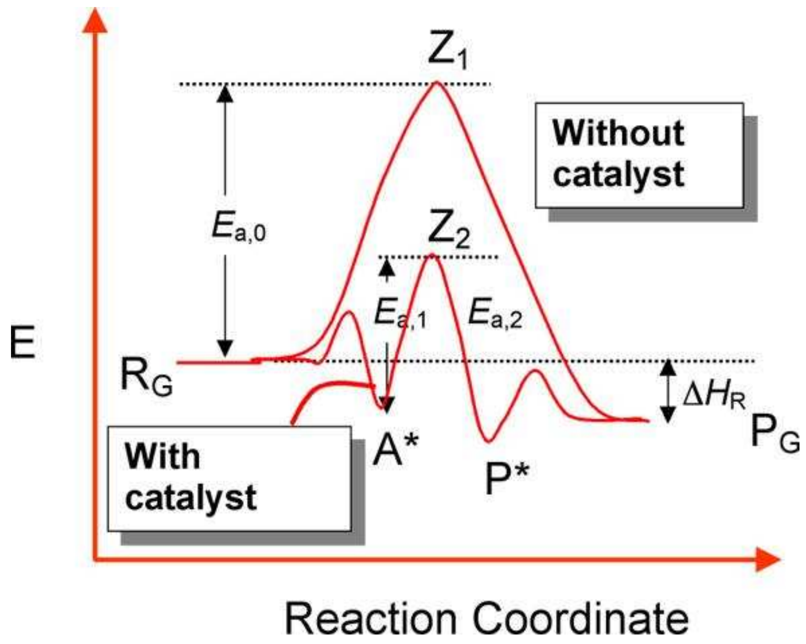

Figure 1 – Energy profile of catalyzed and uncatalyzed reactions

Catalysts **do not change the equilibrium position**; they only help the system reach equilibrium faster.

2. Classification of Catalysis

Catalysis is generally classified into **homogeneous** and **heterogeneous** types, depending on whether the catalyst and reactants are in the same or different phases.

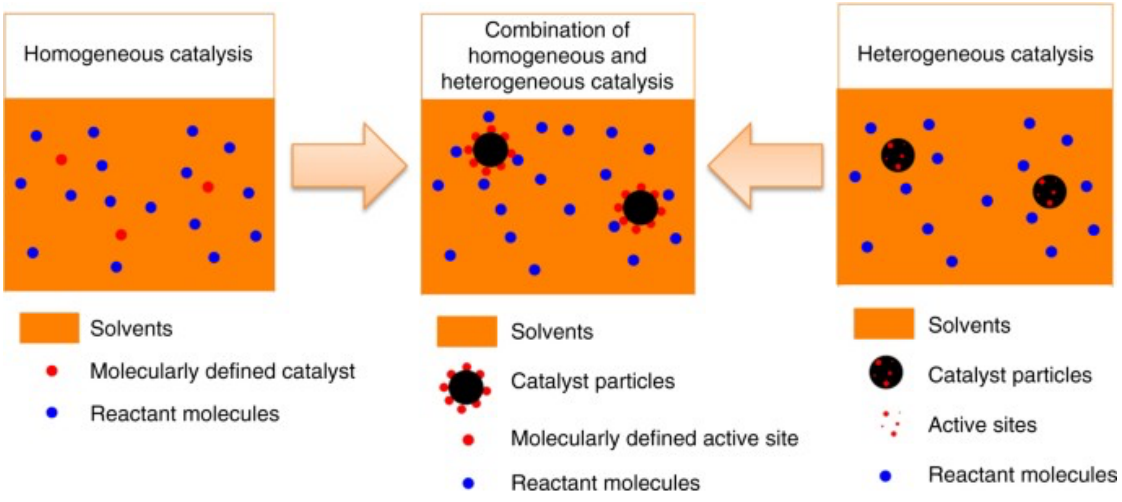

Figure – 2. Construction of homogeneous and heterogeneous catalysis

3. Homogeneous Catalysis

In **homogeneous catalysis**, the catalyst and reactants exist in the **same phase** (usually liquid or gas). The reaction proceeds through the formation of an **intermediate complex** that later decomposes to yield products and regenerate the catalyst.

Example 1:
Oxidation of sulfur dioxide to sulfur trioxide in the presence of nitric oxide (NO) as catalyst:

$$2SO_2 + O_2 \xrightarrow{NO} 2SO_3$$

Mechanism:

$$SO_2 + NO_2 \rightarrow SO_3 + NO$$

$$NO + O_2 \rightarrow NO_2$$

Here, NO acts as a homogeneous catalyst, continuously regenerated in the cycle.

Advantages of homogeneous catalysis:

- Uniform distribution of catalyst throughout the reaction medium.
- High selectivity and controlled reaction pathways.
- Suitable for liquid-phase reactions.

Disadvantages:

- Difficult catalyst recovery and reuse.
- Possible catalyst deactivation due to side reactions.

4. Heterogeneous Catalysis

In **heterogeneous catalysis**, the catalyst and reactants are in **different phases** — typically, solid catalysts interacting with gaseous or liquid reactants. The reaction occurs on the **surface of the catalyst**, which provides active sites where molecules adsorb, react, and desorb as products.

Mechanism (steps):

1. **Adsorption:** Reactant molecules attach to the catalyst surface.
2. **Reaction:** Bonds are broken and new bonds form between adsorbed species.
3. **Desorption:** Products detach from the surface.
4. **Diffusion:** Reactants and products move to and from the surface.

$$A_{(g)} + B_{(g)} \xrightarrow{surface} AB_{(g)}$$

Example 1: Haber–Bosch process (NH_3 synthesis):

$$N_2 + 3H_2 \xrightarrow{\frac{Fe}{K_2O},\, 400\ ^\circ\text{C},\, 200\ atm} 2NH_3$$

Iron acts as the solid catalyst, with potassium oxide as a promoter enhancing its activity.

Table 1 – Comparison between Homogeneous and Heterogeneous Catalysis

Property	Homogeneous Catalysis	Heterogeneous Catalysis
Phase of catalyst	Same as reactants	Different from reactants
Reaction site	In bulk of the medium	On catalyst surface
Example	Acid-catalyzed esterification	Ammonia synthesis on Fe
Separation	Difficult	Easy
Selectivity	High	Moderate
Catalyst reuse	Hard	Easy

Several factors influence the activity and efficiency of catalysts in chemical reactions. The **surface area** of a catalyst is one of the most important factors because a larger surface provides more active sites for reactants to adsorb and react, increasing the overall reaction rate. The presence of **promoters and inhibitors** also affects catalytic activity. Promoters, such as potassium oxide (K_2O) in the Haber process, enhance the effectiveness of catalysts by improving their surface properties or electronic structure. In contrast, inhibitors or poisons, such as carbon monoxide (CO) that deactivates platinum catalysts, reduce catalytic performance by blocking active sites.

Temperature and pressure must be carefully optimized, since higher temperatures generally increase reaction rates but may also lead to catalyst deactivation or undesirable side reactions. Similarly, pressure affects gas-phase reactions and can shift the equilibrium position according to Le Chatelier's principle. Finally, **catalyst poisoning** occurs when impurities or by-products strongly adsorb onto the catalyst surface, blocking active sites and reducing efficiency. Maintaining catalyst purity and appropriate reaction conditions is therefore essential for sustained catalytic activity.

Questions for Self-Control

1. Define catalysis and explain how catalysts increase reaction rates.
2. What are the main differences between homogeneous and heterogeneous catalysis?
3. Describe the steps involved in heterogeneous catalytic reactions.
4. Write examples of industrial processes using solid catalysts.
5. What factors influence the efficiency of a catalyst?
6. Explain how catalysts are used in environmental protection.

Literature:

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