Chemical Reaction Engineering - II
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Module - 1
Lecture - 2
Introduction to Catalysis and Catalytic Processes

Hello. We started in the last lecture by looking at what is the history of catalyst and the catalysis process and what are its potential implications in the world market. In today's lecture, we will define what a catalyst is and we will discuss what is meant by a catalyst and how does it affect the chemical reaction.

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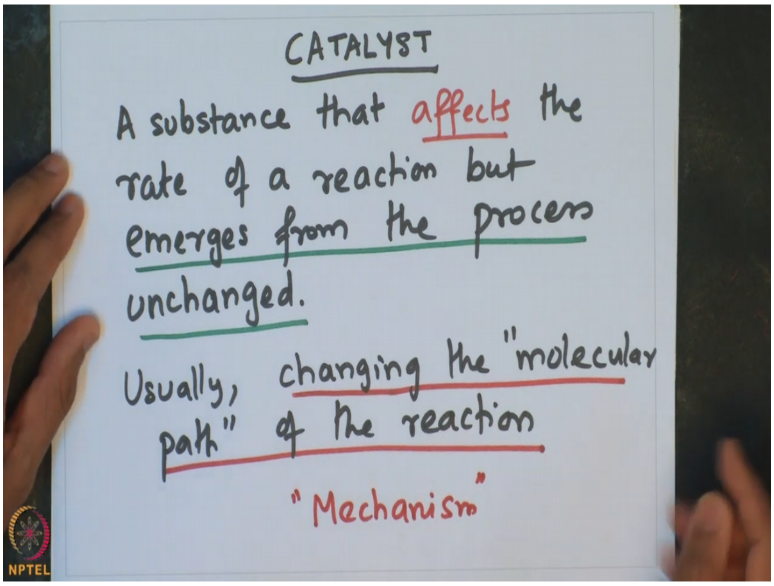

CATALYST

A substance that affects the rate of a reaction but emerges from the process unchanged.

Usually, changing the "molecular path" of the reaction

"Mechanism"

So, a catalyst, it is a substance that affects the rate of a reaction but emerges from the process unchanged. So, it is important to note that the catalyst actually emerges from the process unchanged. It is very important to note that it actually emerges unchanged and it is not really is not consumed when the process is actually happening. Now, that does not necessarily mean that the catalyst is not participating in the reaction.

It may happen that the catalyst is participating, but eventually after the reaction is completed it actually emerges from the process completely unchanged. Usually, this happens by changing the molecular path of the reaction. Usually, the catalyst actually changes the molecular path of the reaction. That is, it essentially changes the mechanism by which a particular reaction actually happens.

So, let me repeat. Catalyst is the one that actually affects the rate of the reaction but emerges from the process completely unchanged. And the way it actually affects the chemical reaction, affects the rate of the reaction is basically by changing the molecular path that the reaction actually takes in order to reach to the product, product stream or product form. And this essentially refers to the fact that it actually plays with the mechanism of the reaction that is actually governing the chemical reaction of taking the species, which is basically the reactants into the products. Let us take a specific example of hydrogen and oxygen.

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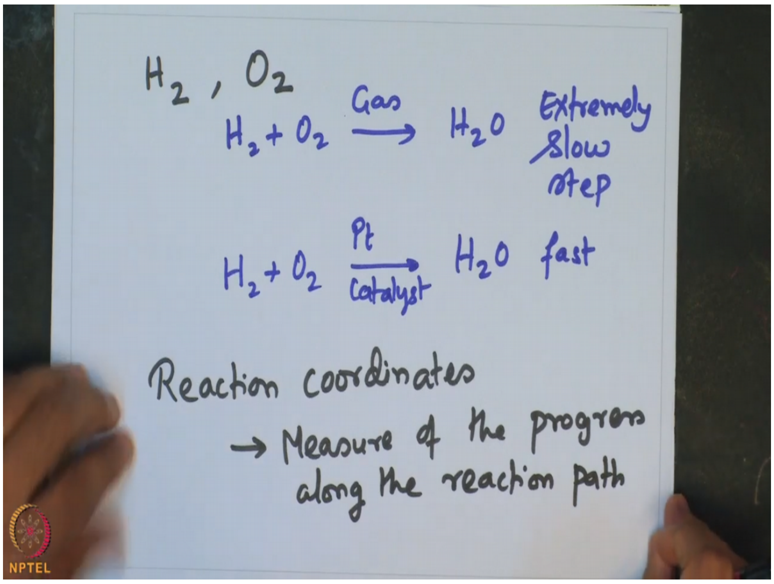

H_2 , O_2

$H_2 + O_2 \xrightarrow{Gas} H_2O$ Extremely slow step

$H_2 + O_2 \xrightarrow[Catalyst]{Pt} H_2O$ fast

Reaction coordinates

→ Measure of the progress along the reaction path

Under normal conditions if the hydrogen and oxygen actually comes together, they really do not react that much to form water. It is actually an extremely slow step that water actually does not form when hydrogen and oxygen molecules, they come close to each other in the gas phase. So, one can depict this in the form of a reaction by observing that H 2 + O 2 when in the gas phase is actually an extremely slow process, extremely slow reactions or water just never forms in practical conditions.

On the other hand, if one conducts the same reaction in the presence of a platinum catalyst, water is formed in a rather faster manner. So, the same species which could not form water in reasonable time, because it is actually an extremely slow step. If there was no catalyst, or the reaction was conducted in the gas phase; when there is platinum catalyst present, the hydrogen and oxygen molecule actually will fastly form water.

And so, presence of the catalyst, clearly you can see that the, it affects the reaction by changing the speed with which the reaction is actually occurring, the step is actually occurring. Now, this can be captured in a slightly different manner, by looking at the reaction coordinates, which is a measure of the progress along the reaction path. So, if I now look at this reaction in the reaction coordinates or the measure of the progress along the reaction path.

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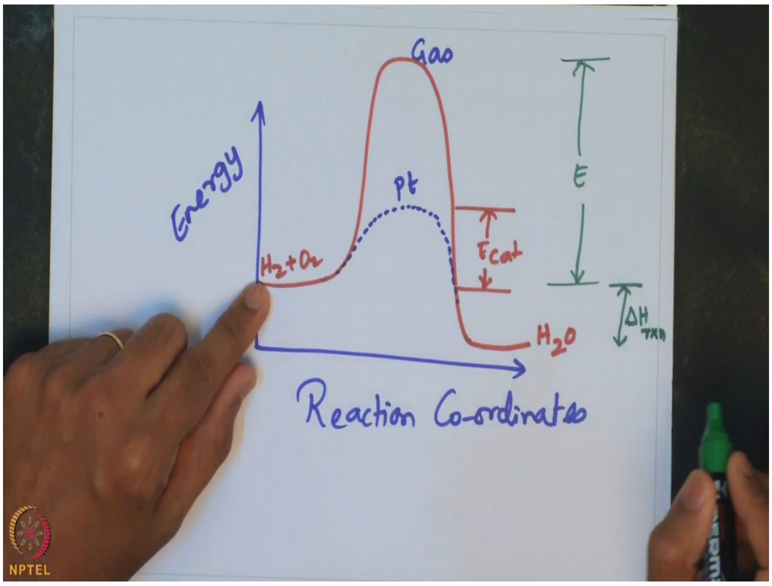

If this is the reaction co-ordinate and let us say that this axis has energy required. And if hydrogen and oxygen, let us say are present here. And energetically, let us say water is present at this level. Then under normal conditions where gaseous phase, the reaction is conducted under the gaseous phase. Then hydrogen and oxygen has to cross an energy barrier and in order to form the products.

So, now we can represent this energy barrier as a hill, where this is the energy that is required for the reaction to occur, if it is in a gas phase. If the reaction is conducted in a gas phase, then this difference in the energy state of the peak of the barrier versus the, or peak of the hill, – what is the energy or at which the reactants are present; that difference is what is called as a, an activation energy.

On the other hand, in the presence of the catalyst, what happens is that the catalyst actually enables reducing this barrier or reducing the activation energy. So, the hill is now reduced in the presence of, let us say, a platinum catalyst. And so, the activation energy is reduced and therefore the barrier for these 2 molecules to come together and forming water molecule actually goes down.

And so, the energy required actually is significantly lesser, in order to convert the hydrogen and oxygen molecules into the water form. So, this is a special property of catalyst where it actually enables reducing the activation energy of the catalyst. Now, I can now mark this energy as what is called as the activation energy in the presence of the catalyst. So, clearly, the presence of a catalyst is of phenomenal value or availability of catalyst for a given reaction is of phenomenal value in terms of reducing the energy and therefore reducing the cost of producing a certain product from the given reactants.

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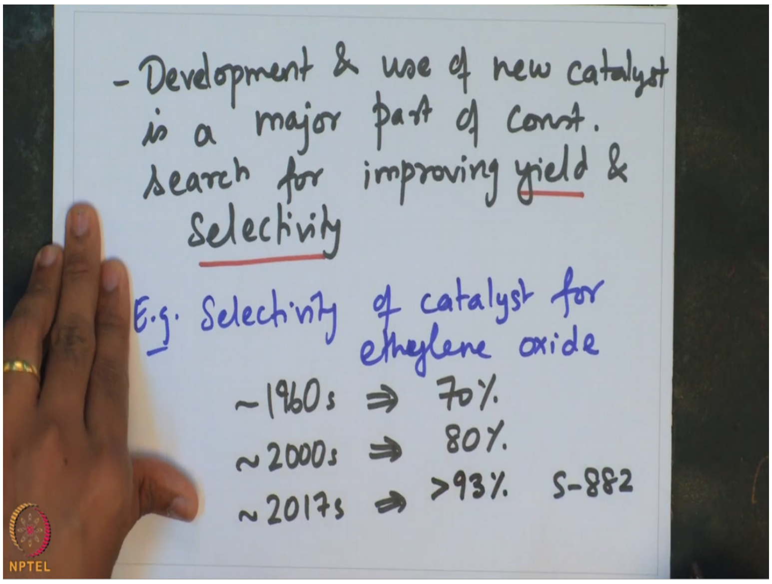

- Development & use of new catalyst is a major part of Const. search for improving yield & Selectivity

E.g. Selectivity of catalyst for ethylene oxide

~1960s ⇒ 70%

~2000s ⇒ 80%

~2017s ⇒ >93%   S-882

So, the development and use of a catalyst, new catalyst, is a major part of constant search, for improving yield and selectivity. Now, this is because the catalyst is known to reduce the activation energy for a given catalyst which is actually taking reactants into a product stream. It actually enables reducing the activation energy for converting the reactants into a products. So clearly, because it is reducing the activation energy, it has a strong, it is likely to have a strong impact on the yield and selectivity of that particular system.

The yield and selectivity of the products that is formed in the presence of the catalyst is certainly is going to be affected by the catalyst itself. So therefore, yield and selectivity is a big issue and if the catalyst can improve the selectivity and yield, it is of great value. So, let us take a specific example where the selectivity of the catalyst, let us look at the example of selectivity of catalysts for ethylene oxide.

So, in the 60s, the activity of the catalyst basically was sufficient only to get about 70% of the selectivity. In the 2000s, new catalysts were manufactured, new catalysts were used to obtain up to 80% selectivity. And today the, today shell actually has, shell has a commercial catalyst called S-882 which actually offers theoretically about 93% selectivity of ethylene oxide. So, the catalyst that is currently used for synthesising ethylene oxide has a great selectivity.

Now, this has a multifold advantage. If the selectivity is very high, then the product stream is actually quite highly enriched with the desired product. And that actually cuts down on the separation processes which is required in order to remove all the unwanted side products that may be present in the products stream. So, therefore the high selectivity catalyst actually has a strong implication in terms of the overall economy of producing that particular product that is desired. So, the typical view, the classical view is that the catalyst actually leads to, so the classical view is that;

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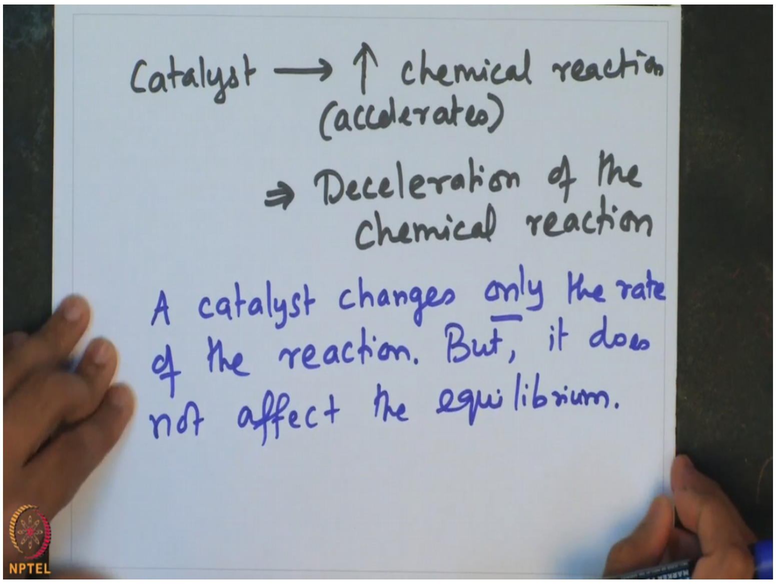

Catalyst → ↑ chemical reaction
(accelerates)

⇒ Deceleration of the
chemical reaction

A catalyst changes only the rate
of the reaction. But, it does
not affect the equilibrium.

The catalyst actually increases the chemical reaction. That is what is the classical, in fact, one should say accelerates the chemical reaction. But that is not necessarily true. It can actually even decelerate the chemical reaction. Even deceleration of the chemical reaction is possible. So therefore, a better view of the catalyst is, a catalyst or a better definition is, catalyst only changes, a catalyst changes only the rate of the reaction but it does not affect the equilibrium of the reaction.

Now, how can we, let us understand this a little bit more. So, if we now look at the energy hill; if we look at the energy hill that is present here. The catalyst actually enables reducing the activation energy between the reactants and the energy state of the reactants and the hill or the peak of the energy barrier. It enables reducing the activation energy which is required for forming the products.

On the other hand, it does not affect the difference in the energetic or the energy states of the reactants and the products which essentially characterises the delta H of that particular reaction. So, delta H reaction which actually is characterised by the difference in the energy states of these 2, is not affected by the catalysts. Which means that the equilibrium properties of that particular reaction are not affected by the presence of the catalyst.

It is only that the activation energy is changed. And thereby it enables accelerating the chemical reaction, accelerating the rate of the, increasing the rate of the reaction or decreasing whichever may be the case; the rate of reaction for that particular reaction of interest.

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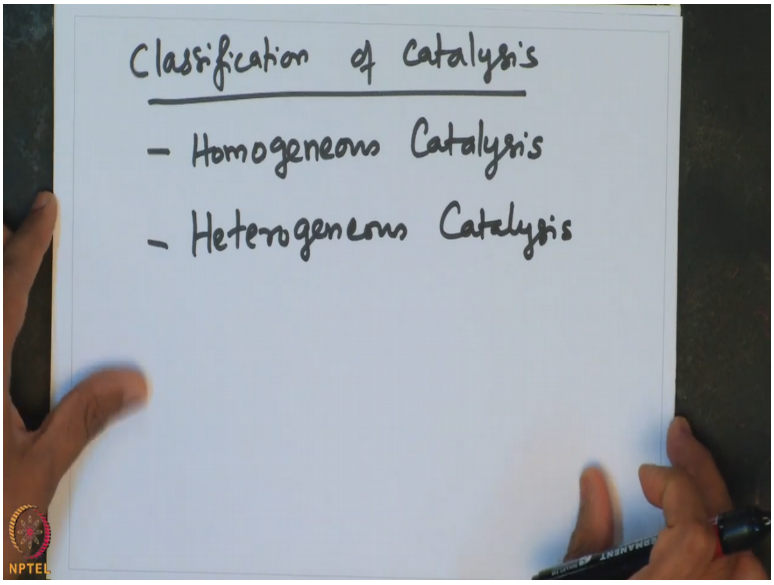

Classification of Catalysis

- Homogeneous Catalysis
- Heterogeneous Catalysis

Let us look at the classification of catalysis. There are essentially 2 types of catalysis or 2 classes of catalysis one may say. One is called the homogeneous, and the other one is the; so, let us first look at what are the characteristics of homogeneous catalysis. And then, we will look at the heterogeneous catalysis.

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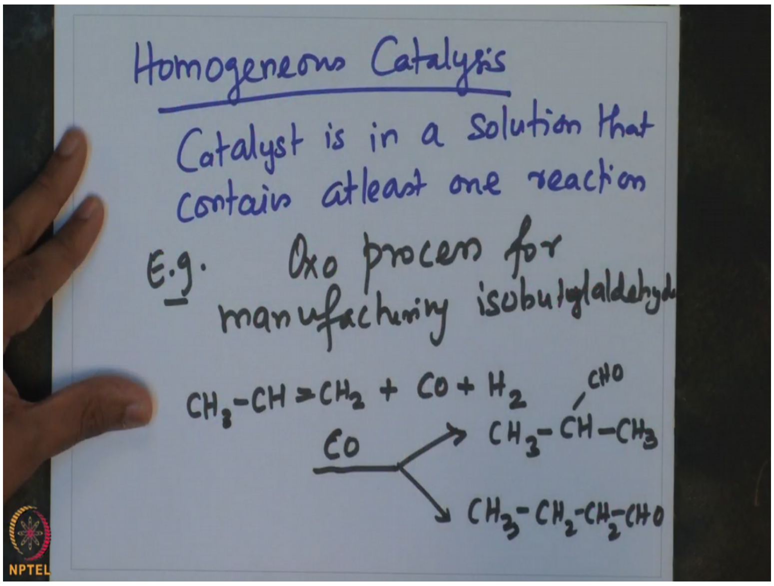

Homogeneous Catalysis

Catalyst is in a Solution that contain atleast one reaction

E.g. Oxo process for manufacturing isobutylaldehyd

$$CH_3-CH=CH_2 + CO + H_2 \xrightarrow{Co} CH_3-\overset{CHO}{CH}-CH_3$$

$$\xrightarrow{Co} CH_3-CH_2-CH_2-CHO$$

So, for the case of homogeneous catalysis, the catalyst is in a solution that contains at least 1 reactant that is participating in the reaction. So, that is the basic premise under which the catalysis process can be called as a homogeneous catalysis where the catalyst is in a solution that contains at least 1 reaction. So, let us take a specific example. Oxo process for manufacturing isobutalaldehyde, is a good example where propylene reacts with C O and H 2 in the presence of a cobalt complex catalyst in the solution phase.

And that leads to isobutalaldehyde and also a byproduct. So, this reaction is actually a homogeneous catalysis process where the reactants and the catalysts, all of these are actually in the same phase. Now in this particular example you will see that it actually leads to the main desired product of isobutalaldehyde and also it leads to a side product of the straight chain butalaldehyde.

So, this is an example of the homogeneous catalysis and reaction typically carried out in super critical fluids have been found to accelerate the reactions and reaction rates greatly. So, that is another example of homogeneous catalysis.

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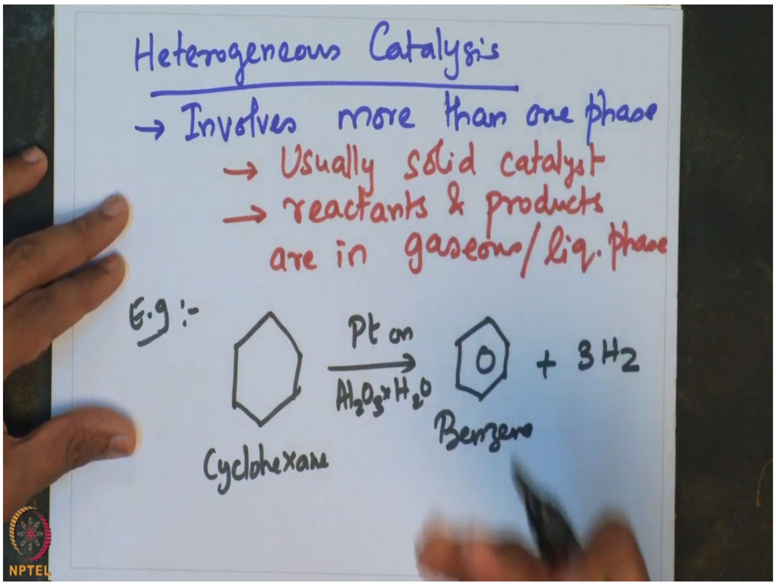

Heterogeneous Catalysis

→ Involves more than one phase
  - → Usually solid catalyst
  - → reactants & products are in gaseous/liq. phase

E.g :-

So, let us look at heterogeneous catalysis. It involves more than 1 phase. For example, usually there is a solid catalyst phase. Usually there is solid catalyst. And the reactants and products are in, or liquid phase. So, there are multiple phases that are actually involved in the catalysis process, where the catalyst is typically present in the solid phase and the reactants and products are actually in, may be in the gaseous or the liquid phase.

So, let us take an example. Let us look at an example. So, cyclohexane; this is cyclohexane on platinum catalyst, platinum on impregnated in alumina, will lead to benzene formation. So, this is actually a heterogeneous catalysis where the platinum which is impregnated on alumina is actually in the solid phase. On the other hand, cyclohexane benzene and hydrogen may be in the gaseous or in the liquid phase depending on the situation.

So, sometimes a reaction picture, mixture is both in the liquid and gaseous phase. Whereas, the catalyst is clearly always in the solid phase. So, there are other several petrochemical industry reactions which are actually using heterogeneous catalysis. And it is more predominant than the homogeneous catalyst because after the catalytic process it is much easier to separate out the product stream and the reactants because the product stream and the catalyst because the catalyst is actually in the solid form.

And therefore, it reduces the separation cost and so on and so forth. So, heterogeneous catalyst is much more prevalent and common than, when compared with the homogeneous catalysis process itself. So, it is a much simpler method. It is much simpler and easier to separate the product stream from the reaction which actually is very beneficial. So, typically separating the products from the catalyst is very important because the catalyst itself will be a very expensive component.

Most of the catalyst that is manufactured are from noble metals. And so, they are very very expensive. And separation of catalyst from the product stream is actually extremely important. Utmost care is usually taken in order to preserve the catalyst and to ensure that the catalyst is not wasted in the product stream.

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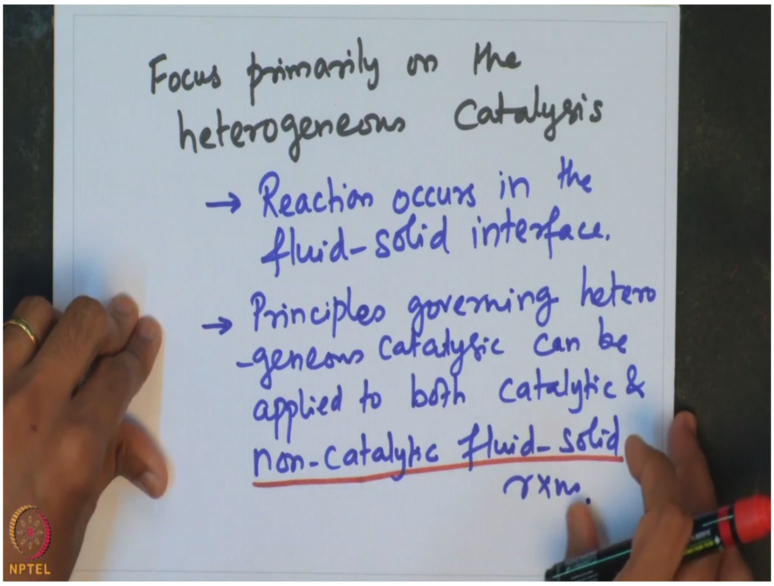

Focus primarily on the heterogeneous Catalysis

→ Reaction occurs in the fluid-solid interface.

→ Principles governing heterogeneous catalytic can be applied to both catalytic & non-catalytic fluid-solid rxn.

So, in this course, we will focus primarily on the heterogeneous catalysis process. Now, the heterogeneous catalysis process, typically the reaction occurs in the fluid-solid interface. So, note that the heterogeneous catalysis, the catalyst is actually in the solid phase. And the fluid which actually comes from bulk which is actually present around the catalyst, they come in contact with the solid interface where the catalyst is impregnated.

And because the catalyst is actually in the solid phase the reaction actually happens at the location where the fluid and the solid meet. That is the interface fluid-solid interface is where most of the reaction is actually happening. And so, characterisation of the fluid-solid interface and understanding what happens at the interface is very crucial to quantitate and design heterogeneous catalysis process.

So, the principles that are developed governing heterogeneous catalysis can be applied to both catalytic and non-catalytic fluid-solid reactions. So, we will be seeing in the future, how to quantitate non-catalytic systems, how to look at non-catalytic fluid-solid multiphase systems, how to look at the reactions that are involving non-catalytic systems where fluid and solid interface becomes important. So, there are several other types of heterogeneous systems.

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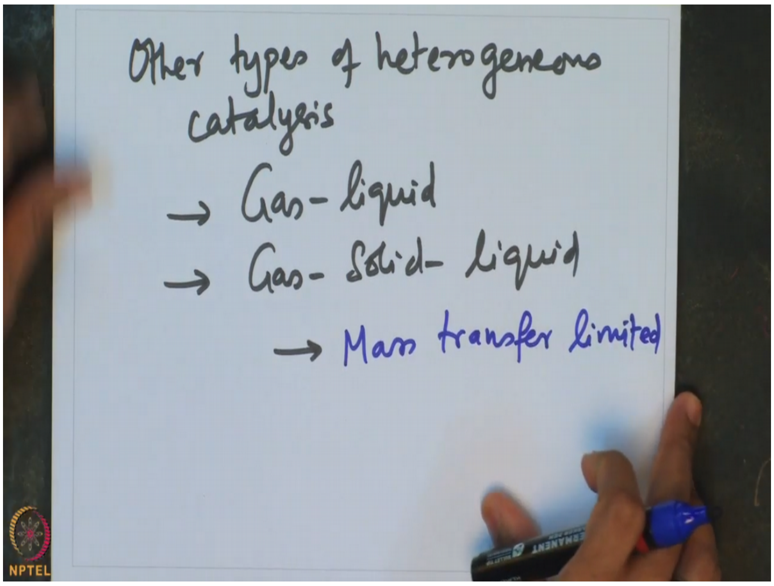

Other types of heterogeneous catalysis

- → Gas-liquid
- → Gas-Solid-liquid
  - → Mass transfer limited

There are other types of heterogeneous catalysis. For instance, there may be gas-liquid systems where the catalyst may be in the liquid form and the reactant stream may be in the gas phase. And the product also may be in the gas phase. There may be 3 phase systems involving gas, solid and liquid phase, where all 3 phases may be involved. And so, typically in these cases, these are, these reactions are typically what is called as mass transfer limited.

We will see a lot more about what is meant by mass transfer limited reactions in one of the future lectures when we talk about the diffusional effects. So, to summarise what we have seen in this lecture.

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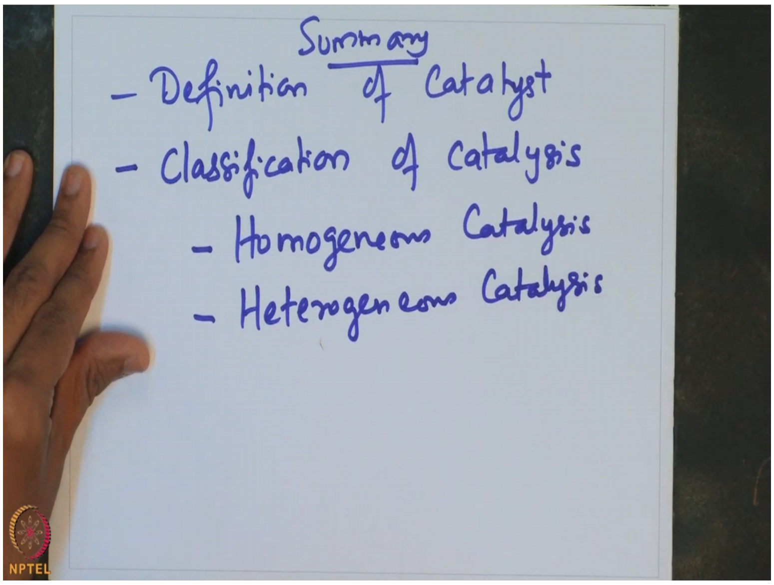

Summary

- Definition of Catalyst
- Classification of Catalysis
  - Homogeneous Catalysis
  - Heterogeneous Catalysis

We looked at definition of a catalyst. We looked at classification of catalysis; homogeneous catalysis and heterogeneous catalysis. So, the take home message for the class is that, whenever there is catalyst which is present, what catalyst does is, it essentially reduces the activation energy which is required for the reaction to happen in the absence of the catalyst. It reduces the activation energy and that thereby it actually facilitates the reaction to happen or for taking the converting the reactant stream into product stream.

Now, while reducing the activation energy it does not change the equilibrium of the reaction. For example, it does not change the delta H reaction, which is the difference between the energy states of the products and the energy states of the reactant. It just does not change the equilibrium of that particular reaction. The catalyst only accelerates or decelerates the reaction rate. It does not change the equilibrium. Thank you.