Process Design Decisions and Project Economics

Prof. Dr. V. S. Mohalkar
Department of Chemical Engineering
Indian Institute of Technology, Guwahati

Module - 3
Reactor Design and Cost Estimation
Lecture - 14
Reactor Non Ideality, Residence Time Distribution (RTD) and Types of Chemical Reactions & Catalysts

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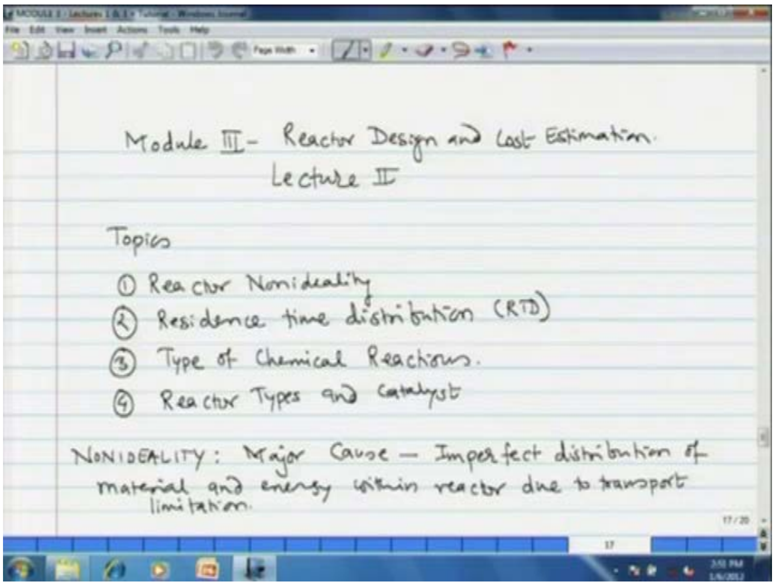

Module III – Reactor Design and Cost Estimation.
Lecture II

Topics

① Reactor Nonideality
② Residence time distribution (RTD)
③ Type of Chemical Reactions.
④ Reactor Types and catalyst

NONIDEALITY: Major Cause – Imperfect distribution of material and energy within reactor due to transport limitation.

Welcome we are in the module of Reactor Design and Cost Estimation. In the previous lectures, we saw some basic aspects of reactor design, we started with the basic reactor principles.

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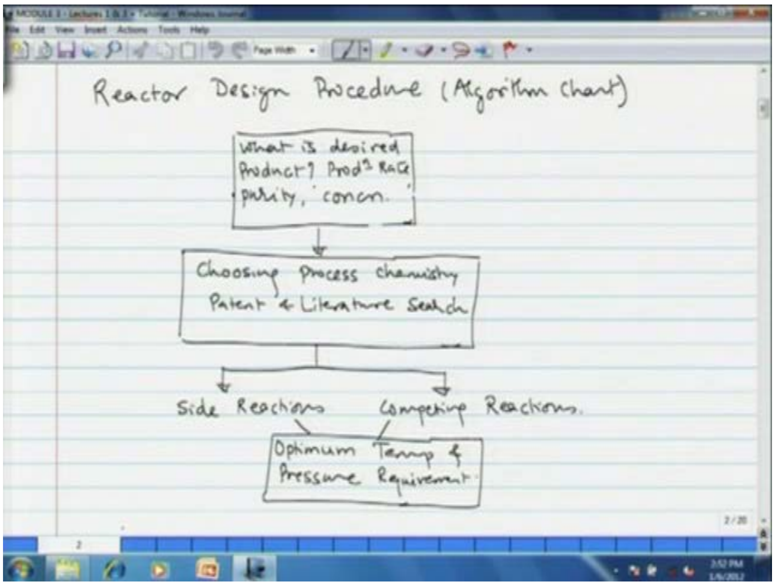

Reactor Design Procedure (Algorithm Chart)

What is desired Product? Prod^n Rate purity, concn.

Choosing Process chemistry Patent & Literature Search

Side Reactions

Competing Reactions.

Optimum Temp & Pressure Requirement

Thereafter, we saw block diagram of the reactor procedure, reactor design procedure or a our algorithm.

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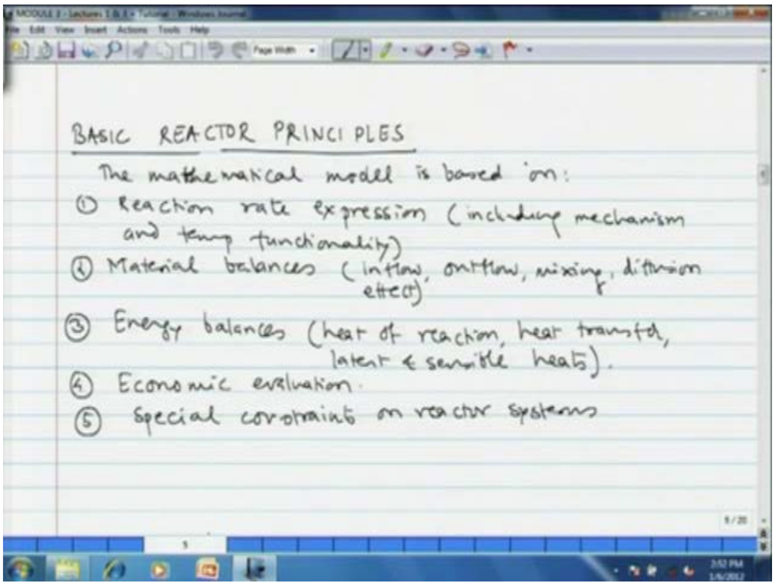

BASIC REACTOR PRINCIPLES

The mathematical model is based on:

① Reaction rate expression (including mechanism and temp functionality)

② Material balances (inflow, outflow, mixing, diffusion effect)

③ Energy balances (heat of reaction, heat transfer, latent & sensible heats).

④ Economic evaluation.

⑤ Special constraints on reactor systems

Thereafter, we tried to develop a simplified or the general expressions for the reaction rate material balance, energy balance, and then we got introduced for about the economic evolution of the reactors and the special constraints on reactor system.

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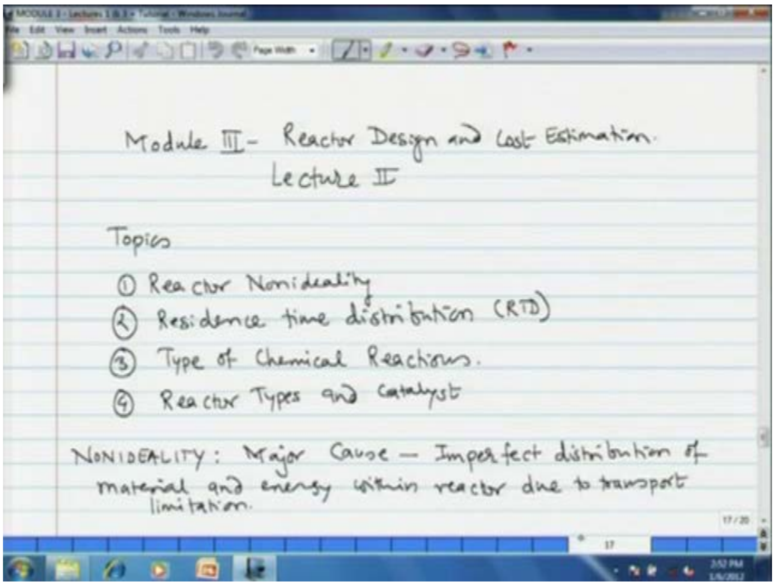

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NONIDEALITY: Major Cause — Imperfect distribution of material and energy within reactor due to transport limitation.

In this lecture, we take further this theme and then see the topics of reactor and non ideality, the residence time distribution, types of chemical reactions and the reactor types and catalyst. The reactor non ideality, the first topic. The major cause reactor non ideality is the imperfect distribution of material and energy with in the reactor due to transport limitations.

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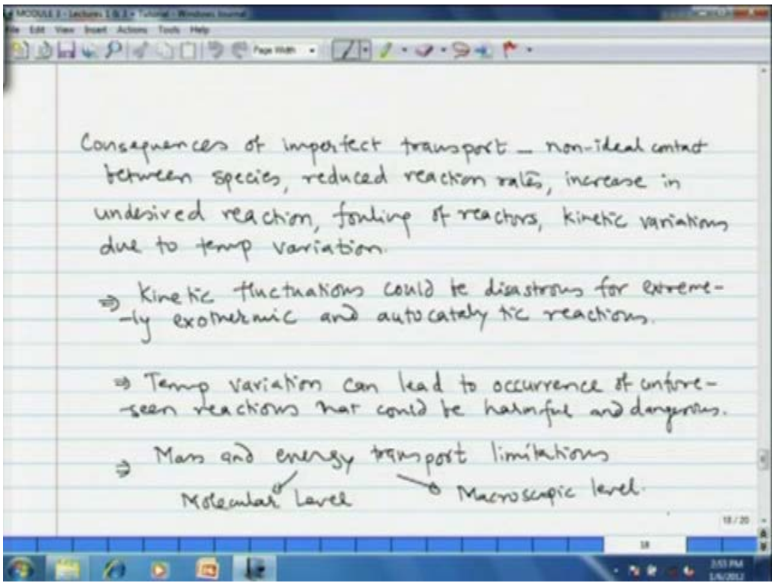

Consequences of imperfect transport — non-ideal contact between species, reduced reaction rates, increase in undesired reaction, fouling of reactors, kinetic variations due to temp variation.

⇒ Kinetic fluctuations could be disastrous for extremely exothermic and autocatalytic reactions.

⇒ Temp variation can lead to occurrence of unforeseen reactions that could be harmful and dangerous.

⇒ Mass and energy transport limitations
Molecular Level — Macroscopic level.

This transport limitations can cause, several undesired effects first of all non ideal contact between the spaces the reduced reaction rate, increased in the undesired reaction, fouling of the reactors, kinetic variation due to temperature variation. Then kinetic variation can further be disastrous for, let us say extremely exothermic or auto catalytic reactions. Temperature variation can lead to occurrence on unforeseen reactions and they, which could not only cause the loss of reactor or they could produce harmful side products and could also pose danger to the sustainable reactor operation. Then the mass and energy transport limitation could be of two types. Firstly, they could be on the molecular level or the microscopic level.

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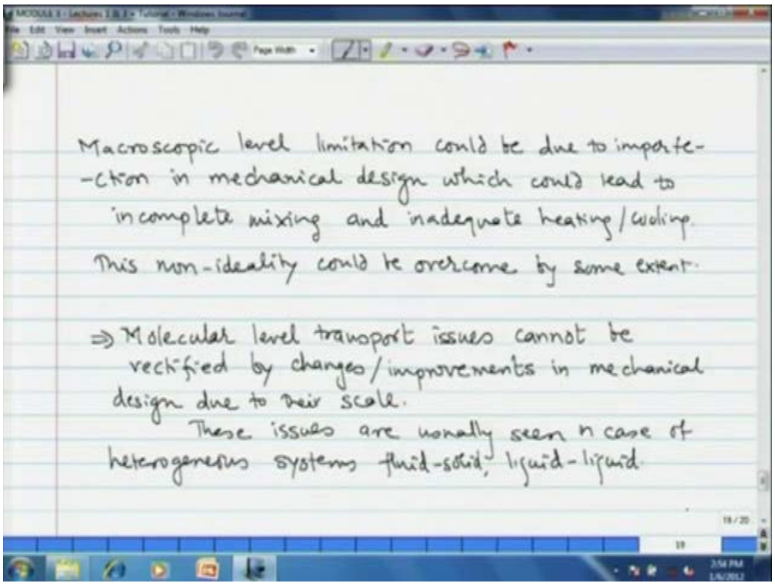

Macroscopic level limitation could be due to imperfection in mechanical design which could lead to incomplete mixing and inadequate heating/cooling.

This non-ideality could be overcome by some extent.

⇒ Molecular level transport issues cannot be rectified by changes/improvements in mechanical design due to their scale.

These issues are usually seen in case of heterogeneous systems fluid-solid, liquid-liquid.

The microscopic level limitations could be due to imperfection in mechanical design of the reactor, which could lead to incomplete mixing and inadequate, heat transport or heating or cooling. Now these kinds of non-idealities could be overcome by some extent or by sometimes completely by modifying the mechanical design of the reactor.

The molecular level transport issues cannot be rectified by these kinds of simple changes or improvements like the change in the mechanical design because the scale on which they occur is extremely small. These types of transport issues can be encountered in fluid solid or liquid invisible systems, like the non-accessibility of the catalytic or unsite of the catalyst, that is an example of a molecular level transport issue.

And some control over these problems can be achieved by changing, let us say the morphology of the system. Like for example changing the catalyst morphology, which could make the catalytic sites, more accessible like for example increase in the pour volume, which could assist the transport of reactant molecule inside the catalyst, then the transport of the product molecule outside the catalyst.

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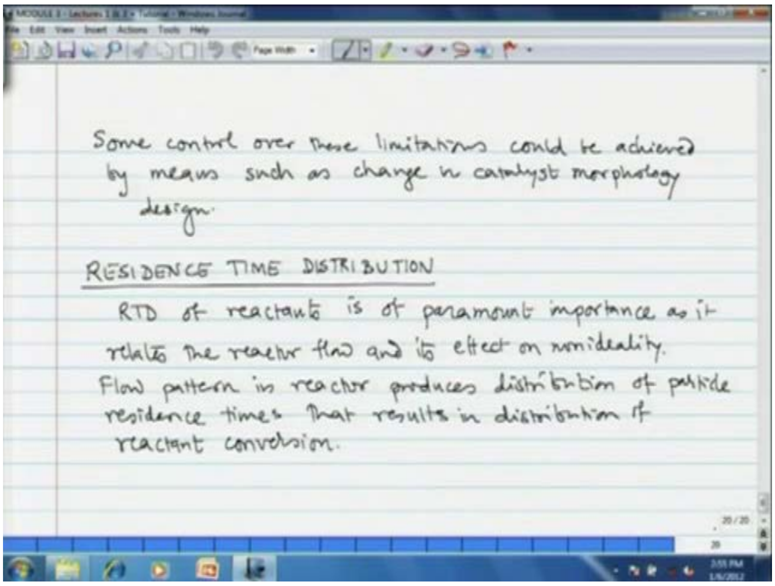

Some control over these limitations could be achieved by means such as change in catalyst morphology design.

RESIDENCE TIME DISTRIBUTION

RTD of reactants is of paramount importance as it relates the reactor flow and its effect on nonideality. Flow pattern in reactor produces distribution of particle residence times that results in distribution of reactant conversion.

Then the next issue is about the residence time distribution, you have already had the detail treatment of the residence time distribution, in the course on reaction engineering. So, here I will give you only the general background, residence time distribution of the reactant typically in a flow reactor is of paramount importance, because it relates the reactor flow and it is effect on non-ideality.

Now the non-ideality especially, let us say for equilibrium limited systems. Deviation from equilibrium, all deviation from the theoretical conversion, could be due to very low residence time in the reactant, in which the complete reaction does not takes occur. Now these effects are more pronounced for slow reactions systems. The flow pattern in the reactor produces a distribution of the particle residence time or fluid element of residence time, that results in the distribution of the reactant conversion.

The flow Pattern in the reactant is very important, whether it is completely plug flow reactor or there is slight back mixing or there is complete back mixing. So, depending on this time residence and time distribution in fact. Determination of time distribution, this topic has also been covered in greater detail in the reaction of engineering course. So, here I give you the basic information, it is usually performed using some treasure material. They are easily derived in a treasure material, treasure enter the reactor system in the same manner as reactants and use the same flow rates as the carrier fluid.

The treasure concentration at the inlet and the exit of the monitored continuously and the collected treasure response data is used to calculate, the residence time distribution pattern in the reactor system. Now is the residence time distribution system a perfect measure of estimating the reactant distribution in the reactor, no there are some limitations like for example. A duplication of treasure response, treasure may not be a unique model of flow pattern with in a reactor system.

Still the several reactor arrangement may yield, the same residence time distribution response for example, if you have the series of CSTRS that may produce, the same RTD pattern as in case of the plug flow reactor. So, you should not use the residence time distribution data in it is completely on it is own. It has to be supported with other element limitation on the production of the unique flow pattern limits the use of the treasure predicted RTD, to simple first order reaction or with relatively constant kinetic constant.

So provided these constant are satisfied reactor is first order reactor and the kinetic order is not going to change much with the concentration temperature etcetera. In that case RTD measurement could be the useful guide design of reactor. How the non ideality in the reactor could be emulated or stimulated. Use of the ideal reactor model, to emulate non ideality model is both simple and useful. This pictoriaology tries to fit an ideal reactor system, to the actual reactor by examining the result of the fluid test in the design reactor.

And enters the ideal reactor model are then arranged in combination to produce, the same result as that of the non ideality reactor. And thus non ideality could be accounted for to some extent. An example in this category is the bimos classification, in which complete carbon conversion does not occur. So, what it usually done is some restriction is put on the carbon conversion and then the simulation is carried out. Assuming equilibrium conversion of other elements and then the reactor factors are estimated and the other gives the difference between, the ideal producer gas.

That can be obtained by complete conversion of or the hundred percent conversion of the carbon and the incomplete conversion of the carbon. So, essentially what we are doing, we are putting the restriction on only on the carbon conversion not on the other elements like hydrogen, nitrogen, oxygen and then you carry out the equilibrium calculation as if in a ideal reactor. So, these are some of the methods of estimating the non ideality in a reactor.

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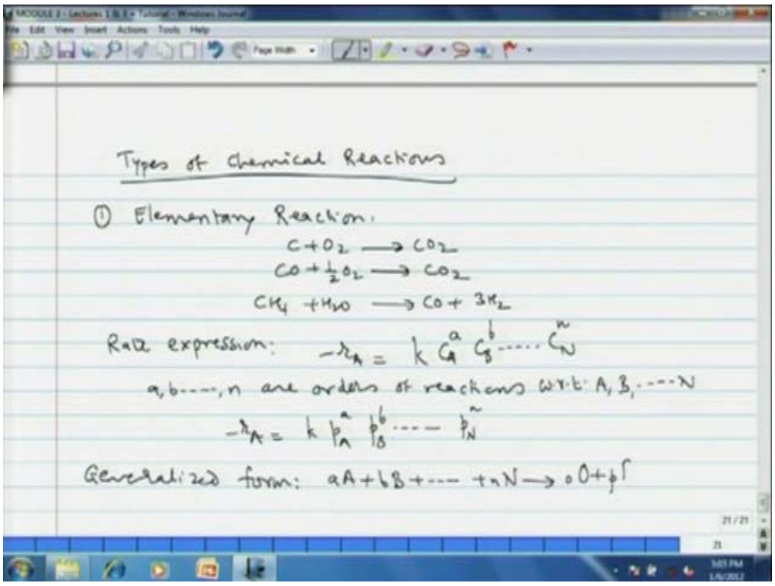

Types of Chemical Reactions

① Elementary Reaction.

$$C + O_2 \longrightarrow CO_2$$
$$CO + \frac{1}{2}O_2 \longrightarrow CO_2$$
$$CH_4 + H_2O \longrightarrow CO + 3H_2$$

Rate expression: $-r_A = k\, C_A^a\, C_B^b \cdots C_N^n$

a, b ----, n are orders of reactions w.r.t. A, B, ---- N

$$-r_A = k\, p_A^a\, p_B^b \cdots p_N^n$$

Generalized form: $aA + bB + \cdots + nN \longrightarrow oO + pP$

Now, let us see the major aspect of the reactor design, that is the type of chemical reaction. Generalize, the reactions or various types of chemical reaction. The first category is that of elementary reaction. For example, carbon plus oxygen giving CO 2 or CO plus half oxygen giving CO 2 or CH 4 plus H 2 O giving CO plus 3 H 2 extremely forming methane so on so forth.

So, these are the simplest type of reactor, in which the observed reactants matches over all with the reactions documentary. Here the molecules of one or more species one react with molecule of another species to give molecules of third species. And the rate expression in this case can be denoted by simple expressions as follows rate expression, you can use the very simple expression. Rate with respect to A that is reactant constant K CA concentration of A raise to small a, which is order of the order with respect to A CB concentration of B raise to small b, with order of the concentration with respect to reactant b and N.

If you have N number of reactants CN raise to n, where a b n are orders of reaction with respected to a b and space C, that are involved. If it is a gas space reaction then, that you can also write. The react expression in terms of partial pressure pA, were is partial pressure of pA and the order remains however, here pA is to a pB were as to pN as to n. So, these are the simplest type of reaction, we can write, generalize form of such reaction aA plus bB plus nN giving oO plus pP like that I can give you.

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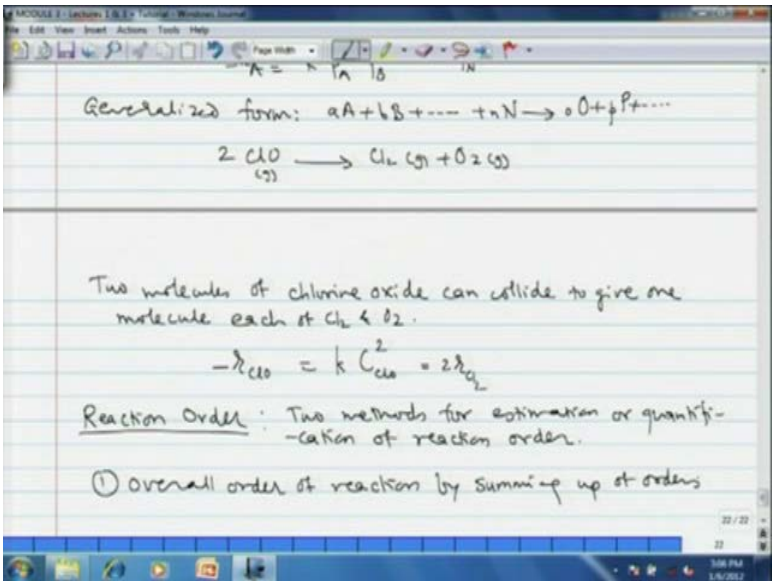

Generalized form: $aA + bB + \cdots + nN \rightarrow oO + pP + \cdots$

$$2\,ClO_{(g)} \longrightarrow Cl_2\,(g) + O_2\,(g)$$

Two molecules of chlorine oxide can collide to give one molecule each of Cl_2 & O_2.

$$-r_{ClO} = k\,C_{ClO}^2 = 2r_{Cl_2}$$

Reaction Order: Two methods for estimation or quantification of reaction order.

① overall order of reaction by summing up of orders

Very simple example of such another reaction. So, the reaction between chlorine and hydrogen gives Clo gas and which further decomposes to Cl 2 and 2 molecules of chlorine oxide can collide to give one molecule. Each of chorine and oxygen and in this case, the rate with respected to clo minus r Clo can be K C Clo square, which could be 2 time rate with respected to Cl 2. Now a measure quantity here is in the reaction order, there are 2 method for estimating.

The reaction order or let us say the quantification of the reaction order. First is the overall order of the reaction by summing up all the reactants, that are involved in the production of the particular product. Overall order of the reaction by summing up of the orders, with respect to all reactors for a particular product. On the second desecration of the order reaction with respected to the particular basis and this is established from the basis documentary co efficient.

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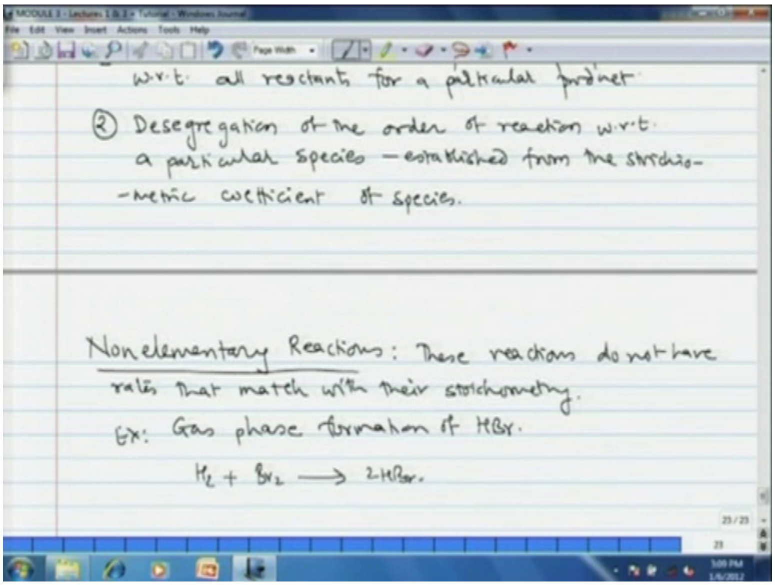

w.r.t. all reactants for a particular product.

② Desegregation of the order of reaction w.r.t. a particular species – established from the stoichio-metric coefficient of species.

<u>Nonelementary Reactions</u>: These reactions do not have rates that match with their stoichiometry.

Ex: Gas phase formation of HBr.

$$H_2 + Br_2 \longrightarrow 2HBr.$$

Then the next reactant size is that of non elementary reaction. Now, these reactions are characterized by the rates that do not match with their documentary. Now how do we how do we go ahead, how do we analyze the non elementary type of reaction. It is often possible to represent non elementary type reaction rate as the group of elementary reaction, simplify the analyses and provide quality to design the non elementary reactions. Now example of non elementary type of reaction is the gas phase formation of hydrogen bromide as established from boardesta, gas phase formation of Hbr. The main reaction are the over all reaction is H 2 plus B 2 gives you 2 Hbr.

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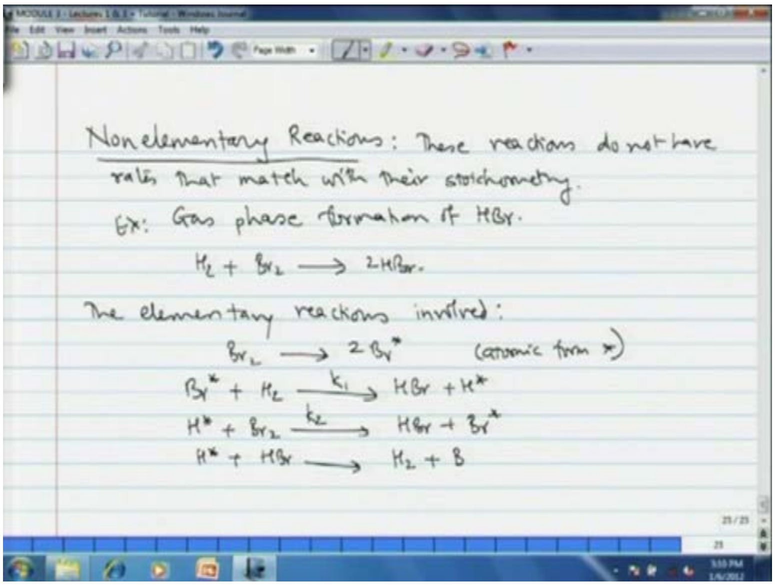

<u>Nonelementary Reactions</u>: These reactions do not have rates that match with their stoichiometry.

Ex: Gas phase formation of HBr.

$$H_2 + Br_2 \longrightarrow 2HBr.$$

The elementary reactions involved:

$$Br_2 \longrightarrow 2Br^* \quad \text{(atomic form *)}$$

$$Br^* + H_2 \xrightarrow{k_1} HBr + H^*$$

$$H^* + Br_2 \xrightarrow{k_2} HBr + Br^*$$

$$H^* + HBr \longrightarrow H_2 + B$$

However, the reaction proceeds through several elementary reactions, first bromine deficits to give atomic bromine. Now that will be denote by super flip star Br star, reacts with hydrogen. Let us say with the constant denoted by K 1 to give Hbr H star. This H star plus bromine further gives again Hbr plus Br star x star plus Hbr give H 2 plus Br star, then 2 atoms of bromine can combine to give bromine molecule 2 atoms of hydrogen can combine to give 2 molecule of hydrogen. Now, if you assume the concentration of atomic form of bromine and hydrogen remain constant through out this process.

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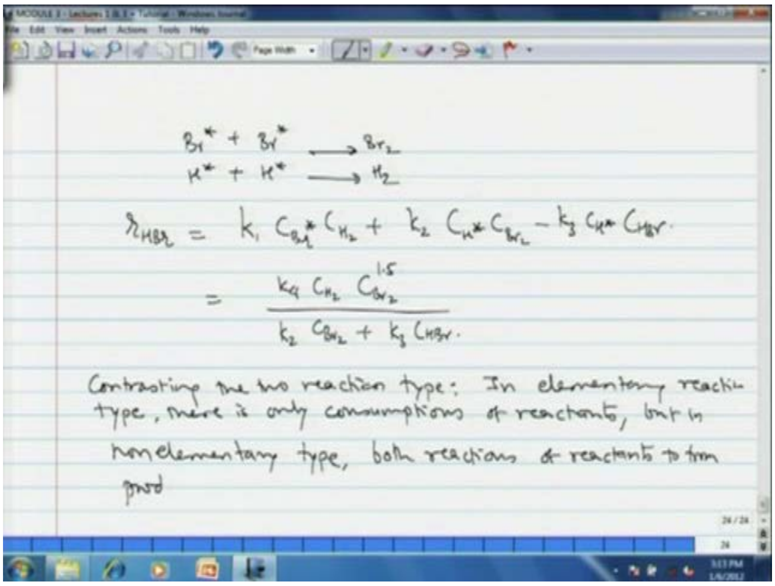

$$Br^* + Br^* \longrightarrow Br_2$$
$$H^* + H^* \longrightarrow H_2$$

$$r_{HBr} = k_1 C_{Br^*} C_{H_2} + k_2 C_{H^*} C_{Br_2} - k_3 C_{H^*} C_{HBr}.$$
$$= \frac{k_4 C_{H_2} C_{Br_2}^{1.5}}{k_2 C_{Br_2} + k_3 C_{HBr}}.$$

Contrasting the two reaction type: In elementary reaction type, there is only consumptions of reactants, but in nonelementary type, both reactions of reactants to form prod

Then this reaction result in the following, non elementary reaction expression, the Hbr the rate of the formation of the Hbr. It can be K 1 Cbr star concentration of bromine atom into C H 2 plus K 2 into C H star plus C B r 2 minus K 3. C H star C H v r, which can be furthered arranged as K 4 C H 2 C B r 2 rest 2.5 divided by K 2 C B r 2 plus K 3 into K 3 into C H B r. How do we contrast the elementary and non elementary types of reaction. In the elementary reaction type. There is only conservation of reactants while in a non elementary reaction type, we often see the reaction of reactant to form product and the reaction of products to form reactant type.

So, that point we note in elementary reaction type. There is only consumption of reactants to form product. But, in non elementary type of reaction, both reactions of reactants to form product reaction are seen. Then there is categories of reversible and irreversible reactions in the module 2. The fluid synthesis, we had seen how we can handle both type of reactions taking H d a as a case study in the hydro dealicalatin process. The first reaction or main reaction of to line plus hydrogen methane plus benzene was irreversible type.

however, the side reaction that is 2 molecule of benzene combine 2 give 1 mole of diesoline was reversible reaction and we saw how we can shift the equilibrium to favourable side. Let us try to treat the same topic in a general way those reaction to in which reaction of reactant to form products is the only reaction are designated as irreversible reaction and the reaction that involve both formation of product from reactant and simultaneous formations reactant from products are designated as reversible reaction, that point we note here.

Reactions in which the reactants only react to form product or designated as irreversibly reaction. And reaction in which both reactants react to form product and products react to form reactant back are reversible reactions.

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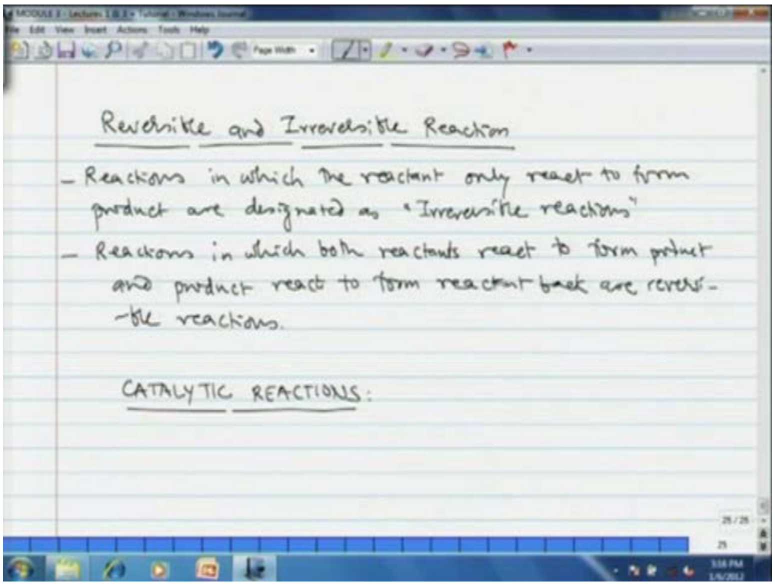

Reversible and Irreversible Reaction

- Reactions in which the reactant only react to form product are designated as "Irreversible reactions"
- Reactions in which both reactants react to form product and product react to form reactant back are reversible reactions.

CATALYTIC REACTIONS:

Than comes the category of catalytic reaction. Now catalytic reactions could be classified on the basis of the phase of the catalyst reduced, if the phase of catalyst is same that of the reactants. Than it is called the homogenous catalyst and if the phase of catalyst is not same or it is different from the phase of the reactants, than it is called hydrogenous catalyst. For fluid face reaction, usually solitary catalysts are used.

Because, solitary continent for contacting gases and liquids and easy to separate as well. Usually, the behavior of the such catalyst is described by the lie boor in saline concept. Here it is assumes that molecules of at least and the one of reactant adsorb on the catalyst surface to react with another reactant. Either gases or soft and then the reaction products desort from the catalyst surface back to the gas phase.

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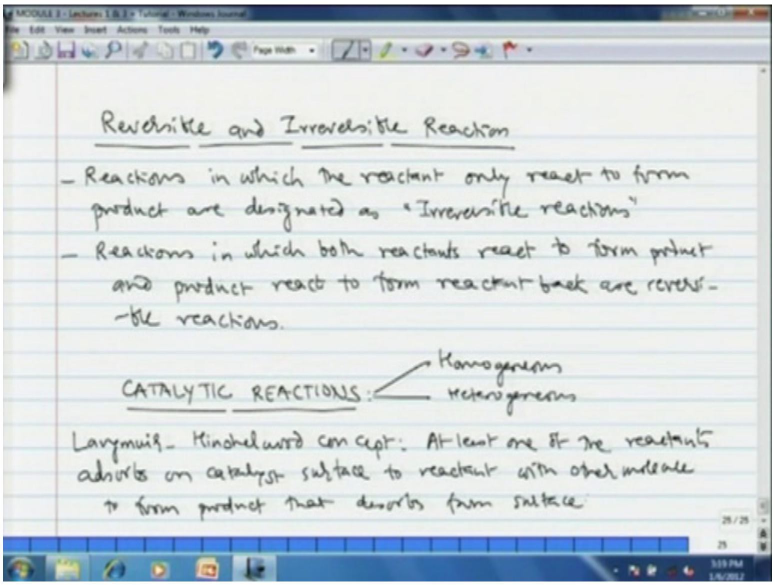

Reversible and Irreversible Reaction

- Reactions in which the reactant only react to form product are designated as "Irreversible reactions"
- Reactions in which both reactants react to form product and product react to form reactant back are reversible reactions.

CATALYTIC REACTIONS: Homogeneous / Heterogeneous

Langmuir- Hinshelwood concept: At least one of the reactants adsorbs on catalyst surface to reactant with other molecule to form product that desorbs from surface.

So, that point be note here, catalytic reaction are 3 types. As I just mention homogenous catalysis, heterogeneous third is biological, but well it can put in the same category. So, we shall say the two categories is redacted 3 homogenous, than line boor in saline concept, at least one of the reactants adsorbs on catalyst surface to react with other molecule to form product, that desorbed from the surface.

So, essentially the catalytic reactions had 3 steps, first the migration of the reactant to the catalyst surface and adsorption, then reactions between adsorb spaces and than desroption and back migration of the products. Now if any of the 3 steps lower than, the others than it is called rate limiting steps or rate controlling steps, the general form the rate expression.

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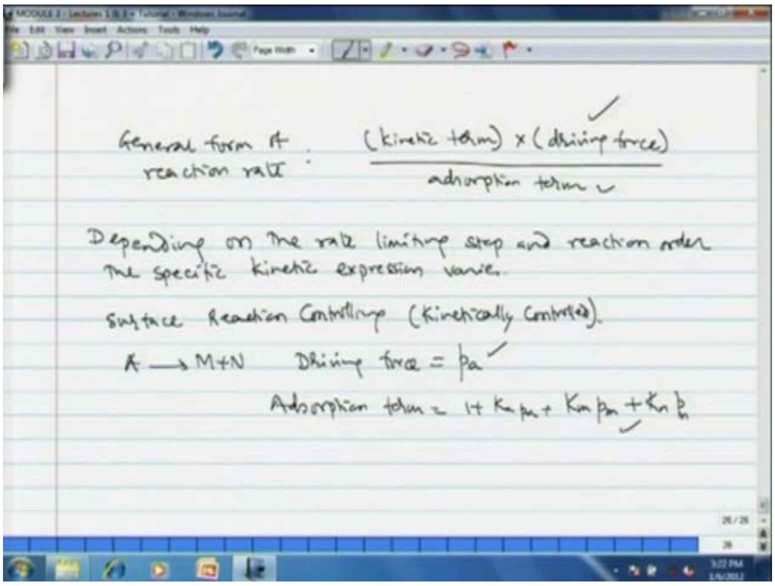

General form of reaction rate : $\dfrac{(\text{kinetic term}) \times (\text{driving force})}{\text{adsorption term}}$

Depending on the rate limiting step and reaction order the specific kinetic expression varie.

Surface Reaction Controlling (Kinetically Controlled).

$A \longrightarrow M+N$ Driving force $= p_a$

Adsorption term $= 1 + K_a p_a + K_m p_m + K_n p_n$

For such reactions is, the cyanotic terms into the driving force divided by the adsorption term, this is the famous lane bore install bore or which is also known as lane bore install bore how then in reaction l h h w module for the catalytic reactions. Now depending on various rate limiting steps and the reaction order the specific equations of the reactions vary, I now give you some typically expression the other expressions, you can find from Paris chemical engineering hand book.

So, that be note depending on the rate limiting steps and reaction order. The specific kinetic expressions varies. Now let us see that what happen in case of surface reaction controlling or kinetically control reactions in such cases, we did not the general expression for the reactions as A going to M plus N. The driving force for such reaction is obviously, the partial pressure of A, but at the adsorption term is one plus capital K a small p a plus capital K b plus small p b.

The capital K m into small p M capital K is the kinetic constant with the respect to p, than capital K n divided by small p n partial pressure of n. So, you substitute this here driving force and adsorbing term, along with the kinetic term with some kinetic constant K 1 or something are than, you get the rate expression for that particular reactions.

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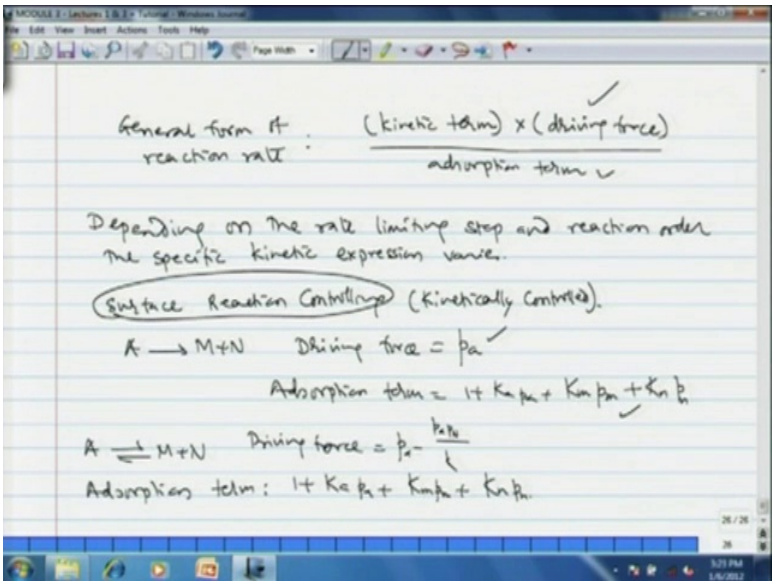

General form of reaction rate : $\frac{(\text{kinetic term}) \times (\text{driving force})}{\text{adsorption term}}$

Depending on the rate limiting step and reaction order the specific kinetic expression varies.

Surface Reaction Controlling (Kinetically Controlled).

$A \rightarrow M+N$ Driving force = p_a

Adsorption term = $1+K_a p_a + K_m p_m + K_n p_n$

$A \rightleftharpoons M+N$ Driving force = $p_a - \frac{p_m p_n}{k}$

Adsorption term : $1+K_a p_a + K_m p_m + K_n p_n$.

Now if the same reaction is reversible, like represent as a going reversible to M plus N, than the driving force if partial pressure of A minus partial pressure of a into a partial pressure of n divided by K, where K is a constant. And adsorption term is 1 plus capital K a p a plus capital K m p m plus capital K n p n. So, this as far as the surface reactions controlling mechanism concerned, where transport is sufficiently fast.

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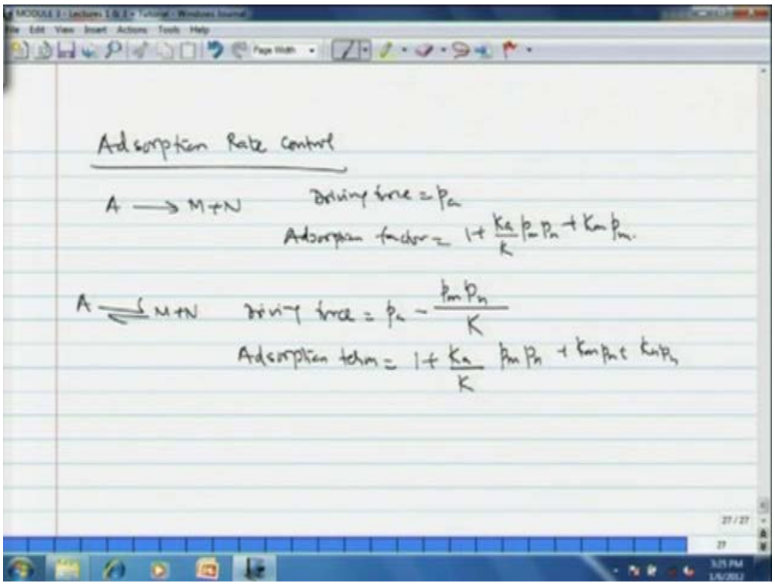

Adsorption Rate control

$A \rightarrow M+N$ Driving force = p_a

Adsorption factor = $1+\frac{K_a}{K} p_m p_n + K_m p_m$.

$A \rightleftharpoons M+N$ Driving force = $p_a - \frac{p_m p_n}{K}$

Adsorption term = $1+\frac{K_a}{K} p_m p_n + K_m p_m + K_n p_n$

Now let us consider a situation in which the adsorption rate controls, the same two type of reactions. First the reversible reaction, it going to impletion. Now in this case, the driving force is equal to per A pressure of a pa. And Arshaarkshan factor is 1 plus K a by capital K into p m into p m plus K m into p m. If it is the revelseable reaction A going revelseable M plus N, than the driving force still p a. But now with a corrections minus p m by p n pm minus p n into p n divided by capital K. Capital K is the equilibrium constant and that, the adsorpsten term is equal to 1 plus capital K a by K p m into p n plus K m p n plus Km np.

So, this is about the catalectic reactions, now another major types of reaction are hensametic reactions, in this reaction involves a reactant under design, that combine reversibly to form a complex. The reaction portion on the reactor portion of the common. Complex is quickly transform to product and the complex splits into the product and the design, which is the released. And now this released design from the complex can go further complex again with another substitute.

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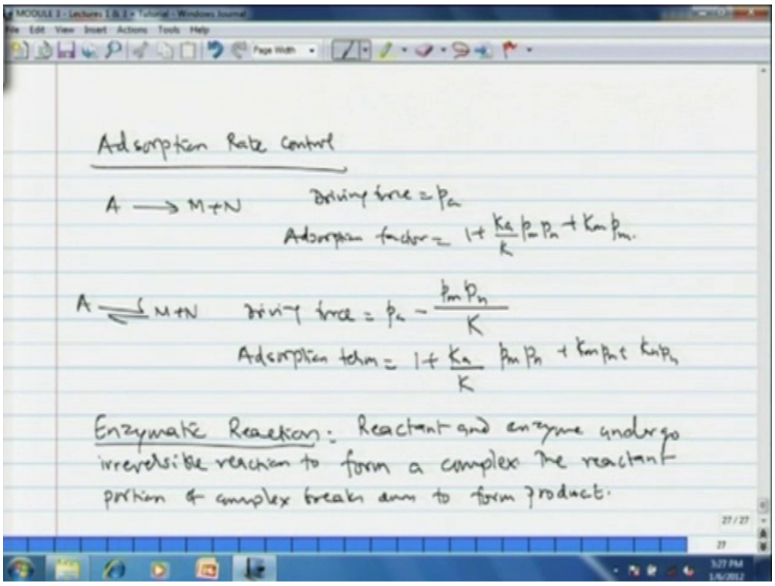

Adsorption Rate control

$A \longrightarrow M+N$ Driving force $= p_a$

Adsorption factor $= 1+\frac{K_a}{K}p_m p_n + K_m p_m$.

$A \rightleftharpoons M+N$ Driving force $= p_a - \frac{p_m p_n}{K}$

Adsorption term $= 1+\frac{K_a}{K}\ p_m p_n + K_m p_n + K_n p_n$

Enzymatic Reaction: Reactant and enzyme undergo irreversible reaction to form a complex. The reactant portion of complex breaks down to form product.

Now these general equations, we can write in the very simple way, I just tell you. First, we notes the points, enzymatic reaction or reactant and enzyme undergo here, reversibly process to form a complex and reactant portion of a complex breaks down to form product and enzyme is regenerated.

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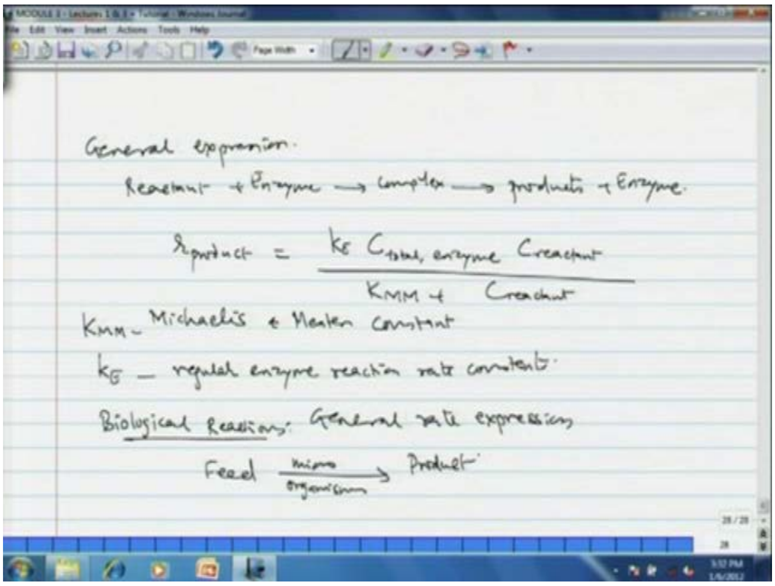

General expression.

Reactant + Enzyme → complex → products + Enzyme.

$$r_{product} = \frac{k_E \, C_{total,\,enzyme} \, C_{reactant}}{K_{MM} + C_{reactant}}$$

K_{MM} – Michaelis + Menten constant

k_E – regular enzyme reaction rate constants.

Biological Reactions: General rate expressions

$$\text{Feed} \xrightarrow[\text{organism}]{\text{micro}} \text{Product}$$

So, we can write the general expressions for this, reactant plus enzyme use complex, which further spreads products plus enzymes. The rate inverse is can we typically written as r product is equal to small k e into central or sorry, that total enzyme concentration enzyme regenerate. So, enzyme is catalyst so we have to consider the total enzyme concentration of course, total enzyme do not still free for because for some enzyme as always cupaid to the sub stated. But, we take into consideration the total consideration is this particular analysis.

Then the concentration of reactant or sub stated, you can call is equal to K m m plus another first K m m is the constant and plus C reactant. This is general form of the earlier expressions. Now K m m is called mica list and maintain constant, this is named after the scientist, who invented this particular invention mica list maintain constant not micas. I am sorry, I will change that spelling maintain micalist make constant, K E is the regular enzyme reaction rate constant.

Now the fourth categories of reaction is that the biologically reactions, example of this type are of reaction are traditional reaction, such as permeation of sugar to produce ethanol or fermentation to produce penicillin. This reaction most of the time enzymatic reaction only carried out instead of using free enzyme by using micro organism. A biological species, now this species could be again in free for immobilize form depending on coherent sensitive of micro organism, we have to design the process. The product of enzymatic reaction inside micro organism are secreted out and they in some cases may adversely effect growth rate of itself.

For good example of this is the asital buthenol formutation, were the product buthenol itself tries to inhabit the reaction by harming the micro organism, which are producing buthenol. So, that is the speciality of this kind of reaction more micro organism require a period adjustment to a new environment, what is always known as lack period, were the consume were they resume. The regular cycle then the general expression rate expression for biological reaction can be given as follows, that point we note general rate expression feed, through organisms micro organisms, go to product.

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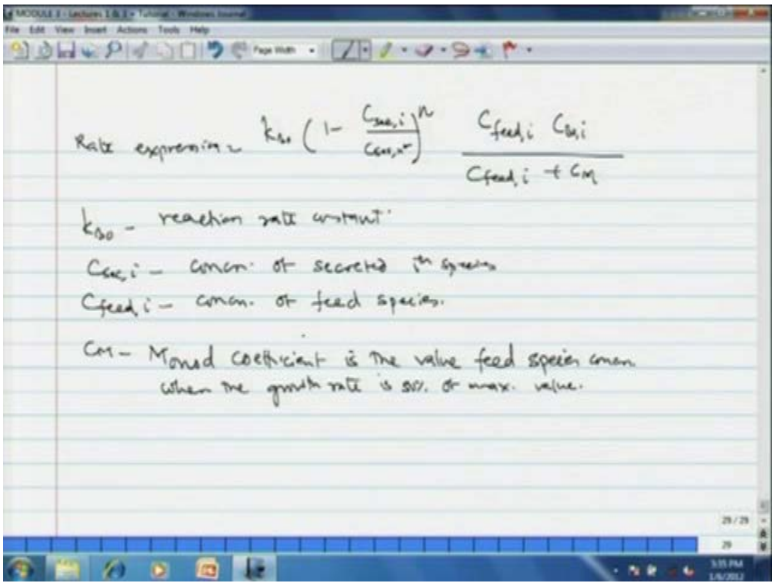

Rate expression = $k_{bo}\left(1-\frac{C_{sec,i}}{C_{sec,i^*}}\right)^n \frac{C_{feed,i}\, C_{bo,i}}{C_{feed,i}+C_M}$

k_{bo} - reaction rate constant

$C_{sec,i}$ - concn. of secreted i^{th} species

$C_{feed,i}$ - concn. of feed species.

C_M - Monod coefficient is the value feed species concn when the growth rate is 50% of max. value.

So, the rate expression is K B o. K is a kinetically constant, B standing for biological 1 minus sec, I divided by Csecsci h star, were h 2 n, into C feed i into C b o i divided by C feed i plus C M. Now I will list all the notation, this expression K B o as I said constant C s e c i or concentration of secreted as I product spices hike product spices, then C feed i is the concentration of feed basis.

C capital M is the mooned co efficient in some colleges bio chemical engineering courses are given elective, were more of this particular expression are treated for different types of fermentation reaction. Now as you might know the mooned co efficient is essential concentration of feed species were the growth rate of micro organism, which 50 percent of its maximum value.

So, that point we note here, mooned co efficient is the value of feed spices concentration, when the growth rate of 50 percent of maximum value. So, that complete our discussion on the reaction types. Now we shall see briefly various type of reactor and catalyst equipment.

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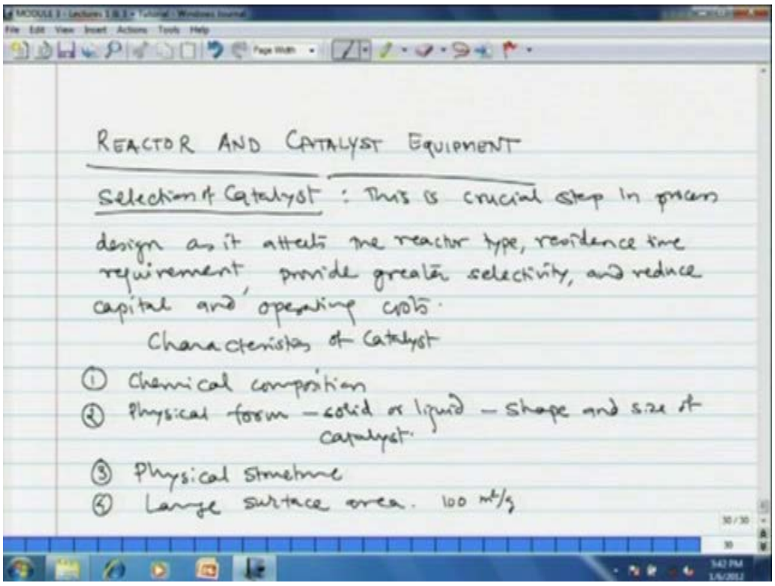

REACTOR AND CATALYST EQUIPMENT

Selection of Catalyst : This is crucial step in process design as it affects the reactor type, residence time requirement, provide greater selectivity, and reduce capital and operating costs.

Characteristics of Catalyst

① Chemical composition
② Physical form – solid or liquid – shape and size of catalyst.
③ Physical structure
④ Large surface area. 100 m^2/g

Many of the industrial reaction are catalyst reaction, were the catalyst is used mostly in the form of solid penile. It could be the reactor, could be fluid bed reactor or moving feed reaction or fixed bed reactor. Those things we are going to see in greater detail later in this topic in this module. But before that we just see what are the factors, that determine the selection of catalyst.

One major factor is the reactant conversion achieved with the catalyst and the product distribution. That the catalyst gives at one what condition the reaction occur, that is also important factor.

So, all this factor we list, selection of catalyst, this is crucial step in process design, as it effects the reactant type residence time requirement, provide greater selectivity, and finally all of this effect the capital and operating cost. Now catalyst selection is not as explicit as the other factor of process design. Catalyst selection is categories as both art and science and expectation, and Scientific analysis is always needed to select the best catalyst, such analysis also form guide line for selection of any other guideline, that company may take over what are the desired of catalyst.

First is chemical constancy, the one element or the compound is key species in the catalyst performance and catalyst also use as several other promoters. Like for example, platinum, palladium, ruthenium catalyst are used for hydro carbon oxidation zinc and zinc chloride are used for the chlorination of the compounds. Zeo lights crystalline aluminum calcite are used, for cracking of the petrol fraction. So, that point we note.

So, the characteristic of catalyst the chemical compound composition, what is the main element and supporting element then second is the physical form of the catalyst whether catalyst is solid liquid. If it is solid what is the shape of the solid? Once, we select catalyst composition and face. The other factor such as catalyst component support have to be established, now there are different kinds of support for catalyst some are hydro Felix, some polymer support like aluminum support so on so…

So, depending on reaction type reaction condition, we have to choose a proper support that will give substance operations for catalyst. Now remember the catalyst is expensive part of the process and replacement of catalyst is not so easy it is also highly expensive. So, we need a catalyst which is ready, which can go on without any operation problem 2 3 year many times, catalyst company agrees to buy back, the catalyst and regenerate and give it back to you. So, if whenever you are choosing the catalyst from, whenever you have the choice of different companies. For catalyst of particular reactant try to look, for this particular alternative whether, the company itself is going to, buy the spent catalyst after certain time 1 year 2 year and give you the regenerated catalyst.

Then the third accept infrastructure of catalyst. Whether catalyst is complete solid or it is a purist solid. The catalyst sides are located on the sites of surface in some cases, the catalyst surface are inside the pore. So, the physical structure of solid catalyst is very important, especially for gas face reaction. Because, it can cause mass per limitation. Finally, we also like to have as large surface area as possible. Typically, surface area is in the order of 100 meter per square gram, such large area are obtained using solid that contain micro and mason pores. Typical catalyst support in are such as solids laminar silica luminous. Silicate and active catalyst space is usually deposited on the surface of the support. The reactant transport to and product from reaction site catalyst can limit, the effectiveness or utilization of the catalyst.

So, you have already delft, with the effective the catalyst effectiveness factor in the module of chemical factor engineering, what is the concentration of the reactant in the bulk. And what is the concentration in the catalyst pore, that ratio decides the effectiveness factor of the catalyst. The reactant rate constant and defection co efficient, there relative also effect the utility of the particular catalyst. In case the savic entrance, which the reactant molecule are larger, than the pore than increase, the co efficient by changing the co efficient of the more accessible. Then finally, the stability of the catalyst is also important that point we note catalyst of course, by increasing twice you reduce the area. But, you make catalyst site.

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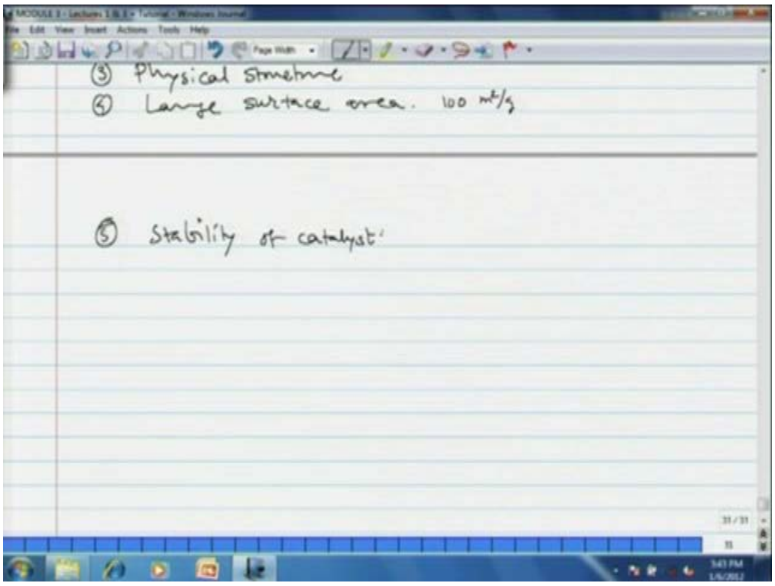

③ Physical Structure
④ Large surface area. 100 m²/g

⑤ Stability of catalyst.

Stability of catalyst as I just mentioned some reaction could be harsh high temperature high pressure. So, your catalyst support should be strong enough to bear all the thermal variations pressure variations, various stress and impose over the catalyst. There are 2 types of stability, one is the mechanical stability and another is chemical stability the mechanical stability, that I just mentioned catalyst support should be strong enough, it should not sinter the catalyst should not get fragmented. Because, of thermal variation and the second stability is the chemical stability, which is present in the impurity and the poisons. Usually the sulphur contain compound such as H 2 S can strongly absorb reaction site and block them in many organic reaction catalyst coated with carbon deposit, which also reduce there activity.

So, the ability to regenerate the activity of the catalyst is very important protection of catalyst, from exploration to poison is extremely essential, you have to scrub the gaps. Whenever you are using still gas H 2 S impurity, you have to scrub. The gaps reduce the concentration of H 2 S 2 ppm or sometimes ppb level. The catalyst support must also have sufficient physical strength as I just mentioned and then, it should sustain extreme operate condition or abnormal operating condition, we if let us say temperature occur in the reactor.

Because of heat transformation limit the catalyst should not get deactivated or fragmented. So, mechanical stability also an important accept. So, that is how we have covered that various topic, in this particular lecture. And in next lecture we shall see the type of reactor and then, the reactor procedure then the reactor cost estimation, and finally, we shall have a problem of reactor design.