Chemical Reaction Engineering - II

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Module - 3
Lecture - 11
Design of Reactors: PBR and CSTR

Friends, let us summarise what we have learnt in the last lecture.

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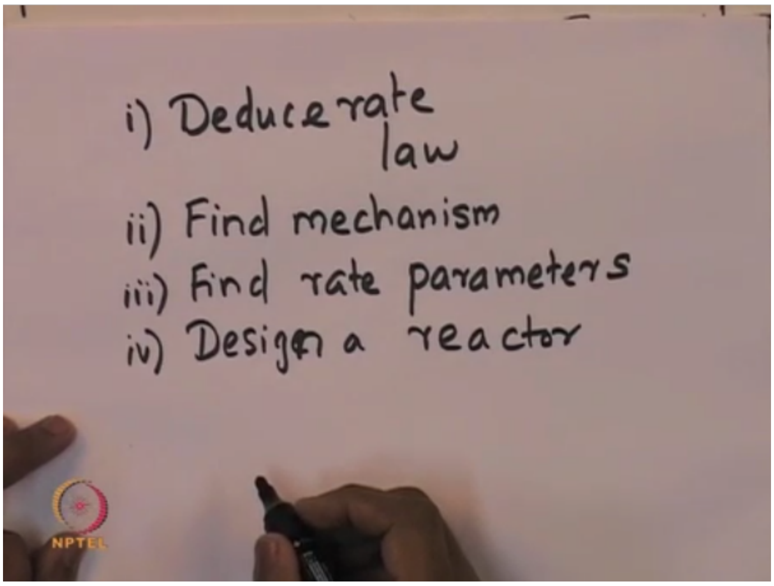

i) Deduce rate law
ii) Find mechanism
iii) Find rate parameters
iv) Design a reactor

So, we have learnt how to, if there is a heterogeneous catalytic reaction, we have learnt how to deduce the rate law from experimental data, deduce the rate law. We have learnt the second step how to find mechanism, how to find the mechanism behind a certain catalytic reaction. And we have found the, for a particular example we found the rate parameters. And then we initiated discussion on how to design a reactor.

In particular, we considered the example of hydro demethylation of toluene on solid mineral catalyst containing a certain material called clinoptilolite and we looked at the experimental data for that particular reaction. And then, we tried to deduce the mechanism and tried to estimate the rate parameters.

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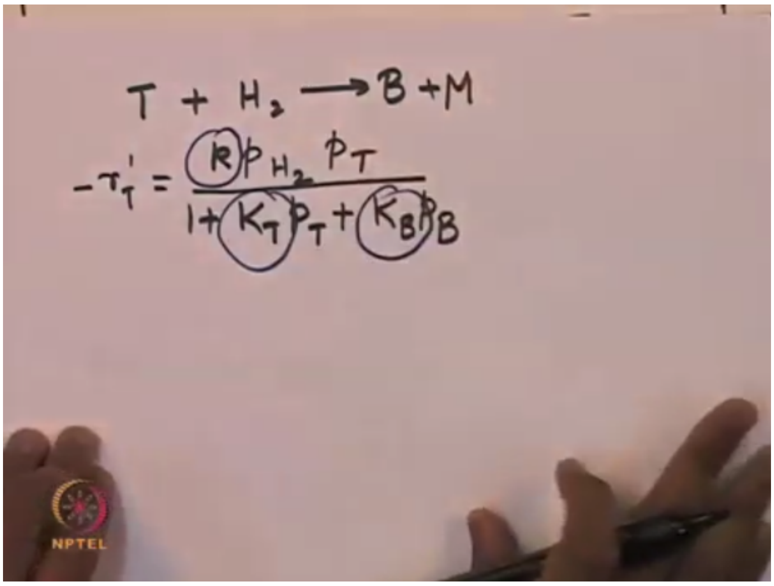

$$T + H_2 \longrightarrow B + M$$

$$-r_T' = \frac{\boxed{k}\, p_{H_2}\, p_T}{1 + \boxed{K_T}\, p_T + \boxed{K_B}\, p_B}$$

We found that for the toluene reacting with the hydrogen leading to benzene and methane formation; so for that reaction we deduce that the rate of the reaction can be represented as the rate of consumption of the toluene can be written as some rate constant k multiplied by the partial pressure of hydrogen multiplied by the partial pressure of toluene divided by 1 + the adsorption constant for toluene multiplied by the partial pressure of toluene + the adsorption constant for benzene multiplied by the partial pressure of benzene.

So, then we use the experimental data in order to perform a linear regression analysis and estimate these parameters k, estimate the parameters k, estimate the parameter K T and also K B from experimental data. Then we initiate a discussion on the design of a reactor using this rate law. So, while designing the reactor we wrote a mole balance and found what is the balance equation that represents the, that captures the conversion in the reactor as a function of the weight of the catalyst.

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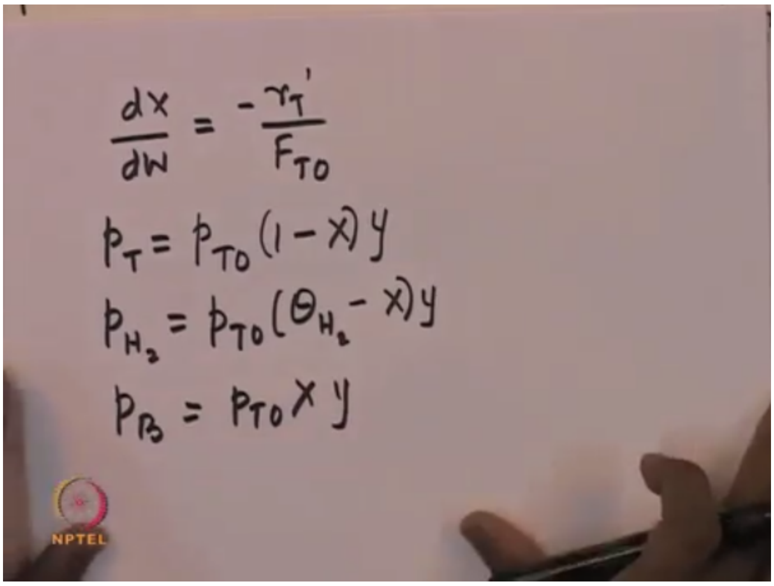

$$\frac{dX}{dW} = -\frac{r_T'}{F_{T0}}$$

$$p_T = p_{T0}(1-X)y$$

$$p_{H_2} = p_{T0}(\Theta_{H_2} - X)y$$

$$p_B = p_{T0}Xy$$

And so, that turned out to be d X by d W. X is the conversion and W is the weight of the catalyst in the reactor = – r T prime divided by F T 0, where – r T prime is the rate at which toluene is actually being consumed in the reaction. And, also F T 0 is the initial feed molar rate of toluene species which is participating in the reaction. We also found that the partial pressure of toluene can actually be expressed as the partial pressure of toluene at the inlet P T 0 multiplied by 1 – the conversion into y which is the mole fraction.

And similarly, for the partial pressure of hydrogen which is expressed as P T 0 into the feed ratio of hydrogen to toluene – the conversion into the mole fraction. And for benzene it will be P T 0 into X into y. So, we will continue from there today. And so, the first exercise is to find out what is this expression for, what is y.

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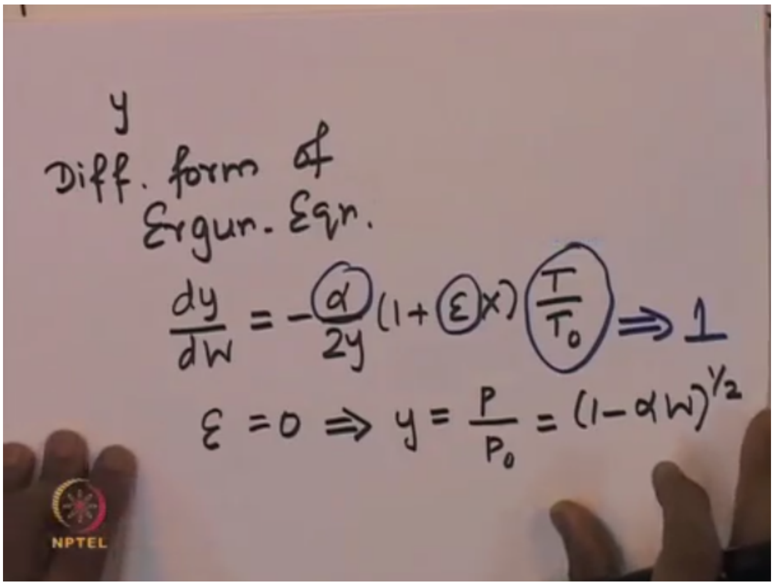

y

Diff. form of Ergun. Eqn.

$$\frac{dy}{dW} = -\frac{\alpha}{2y}(1+\varepsilon X)\left(\frac{T}{T_0}\right) \Rightarrow 1$$

$$\varepsilon = 0 \Rightarrow y = \frac{P}{P_0} = (1-\alpha W)^{1/2}$$

That is, what is the mole fraction? And that can be obtained; what is the relationship of mole fraction and the other and the conversion inside the reactor? And that can actually be found out using the differential form of Ergun equation. And which is, which can be written as d y by d W. That is = – alpha by 2 y multiplied by 1 + epsilon X into T by T nought. Where alpha is the pressure drop parameter. Epsilon is the total fractional change in the number of moles.

And X is the conversion and T is the temperature at that location and T nought is the inlet temperature. If we assume that it is isothermal conditions, then T by T nought is = 1. If you assume that it is a isothermal, the reactor is actually, the reaction is conducted under isothermal conditions, then the temperature in the reactor is same as the inlet temperature of the fluid stream. And therefore, T by T nought will be = 1.

And for the chosen reaction, the epsilon which is the total change in the number of moles because of the reaction is = 0, because the next stoichiometry coefficient is 0. And from here we can solve the differential Ergun equation and obtain the expression for y as a function of the other parameters which is P by P nought = 1 – alpha times W to the power of half, where alpha is the pressure drop parameter and W is the weight of the catalyst.

So, the mole fraction at any location in the reactor will now depend upon how much catalyst is present till that location and the corresponding pressure drop parameter. So now, we can actually plug this into the model equation and then we can attempt to find out what is the conversion as a function of the weight of the catalyst.

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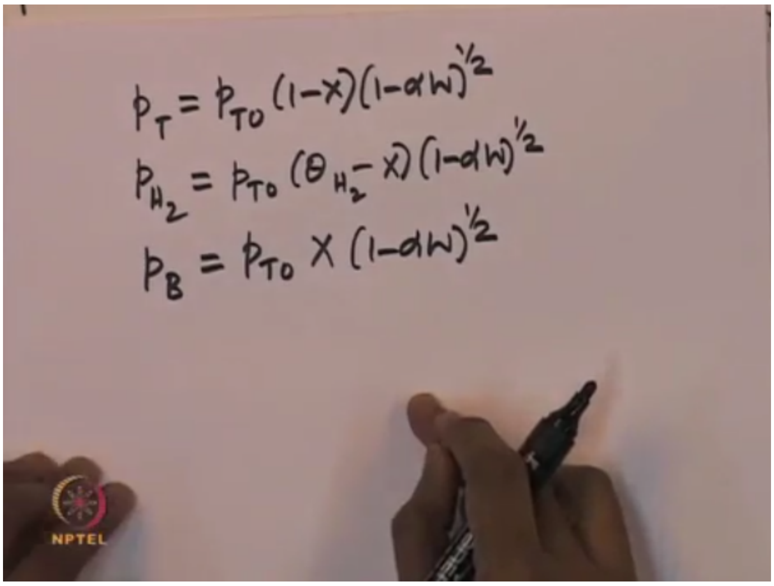

$$p_T = p_{T0}(1-X)(1-\alpha W)^{1/2}$$

$$p_{H_2} = p_{T0}(\Theta_{H_2} - X)(1-\alpha W)^{1/2}$$

$$p_B = p_{T0}\, X\, (1-\alpha W)^{1/2}$$

So, therefore the partial pressure of toluene is now given by P T 0 which is the total partial pressure of toluene at the inlet multiplied by 1 – X which is the conversion into 1 – alpha W to the power of half. And similarly, that of partial pressure of hydrogen is given by P T 0 into 1, theta H 2 which is the feed ratio of hydrogen versus toluene – the conversion into 1 – alpha W to the power of half.

And the partial pressure of benzene is given by P T 0 into conversion into 1 – alpha W to the power of half. So, now we have all the information that we need to solve the equation and so let us look at how to, let us put them all together. So, the model equation that relates the conversion with the weight of the catalyst is given by:

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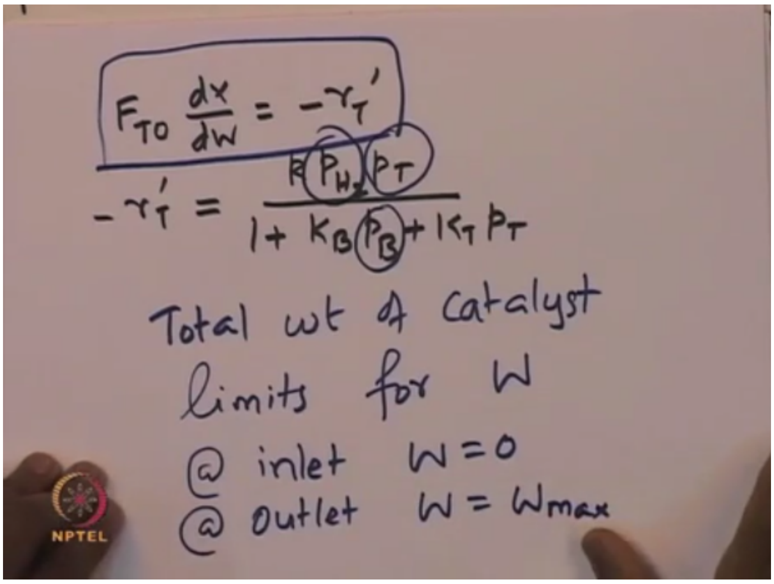

$$\boxed{F_{T0}\frac{dx}{dW} = -r_T'}$$

$$-r_T' = \frac{k P_{H_2} P_T}{1 + K_B P_B + K_T P_T}$$

Total wt of catalyst

limits for W

@ inlet W = 0

@ outlet W = Wmax

F T 0 multiplied by d X by d W that is = – r T prime which is the rate of generation of toluene. And we know from the rate mechanism that the rate of generation is given by K into partial pressure of hydrogen into partial pressure of toluene divided by 1 + K B into partial pressure of benzene + K T into partial pressure of toluene. So now, what we need to know is, what are the limits of the integration.

We know what is, we know the expressions for partial pressure of hydrogen in terms of conversion, we know the expression for partial pressure of toluene in terms of conversion and we know the expression for partial pressure of benzene in terms of conversion. Now, once we know this in order to integrate the only piece of information that is required is what is the total weight of the catalyst in the reactor.

Now, why we need this? Because, we need to, in order to integrate this expression here, in order to integrate the expression which is present here, we need to know what are the limits for the, limits for W which is the weight of the catalyst. So, of course at the inlet the weight of the catalyst is 0. But at the outlet let us assume that there is W is given and by some maximum weight of the catalyst.

Now, how do we find this maximum weight of the catalyst? So, we know the expression for the mole fraction as a function of the weight of the catalyst. So, what we can do is, suppose if we assume that the reactor, the fluid stream exits the reactor at atmospheric pressure.

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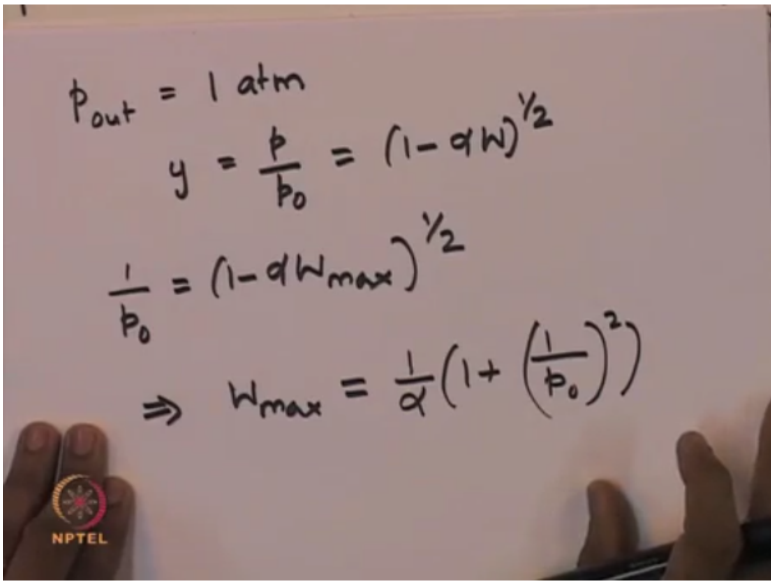

$p_{out} = 1$ atm

$$y = \frac{p}{p_0} = (1 - \alpha W)^{1/2}$$

$$\frac{1}{p_0} = (1 - \alpha W_{max})^{1/2}$$

$$\Rightarrow W_{max} = \frac{1}{\alpha}\left(1 + \left(\frac{1}{p_0}\right)^2\right)$$

So, suppose the pressure at which the fluid stream leaves the reactor is 1 atmosphere, then we will be able to estimate what is the maximum weight because we know the relationship between the mole fraction y which is P by P nought. That is = 1 – alpha times W to the power of half. So, from this expression, we can now substitute the pressure at the exit of the reactor and find out what is the weight of the catalyst in terms of the other parameters.

So, therefore 1 by P nought = 1 – alpha W max to the power of half. So, this means that the maximum weight of the catalyst, if the pressure at the outlet is 1 atmosphere, that will be = 1 by alpha into 1 + 1 by P nought whole square. So, now we have all the required information in order to integrate the model equation. So, let us look at, let us put them all together.

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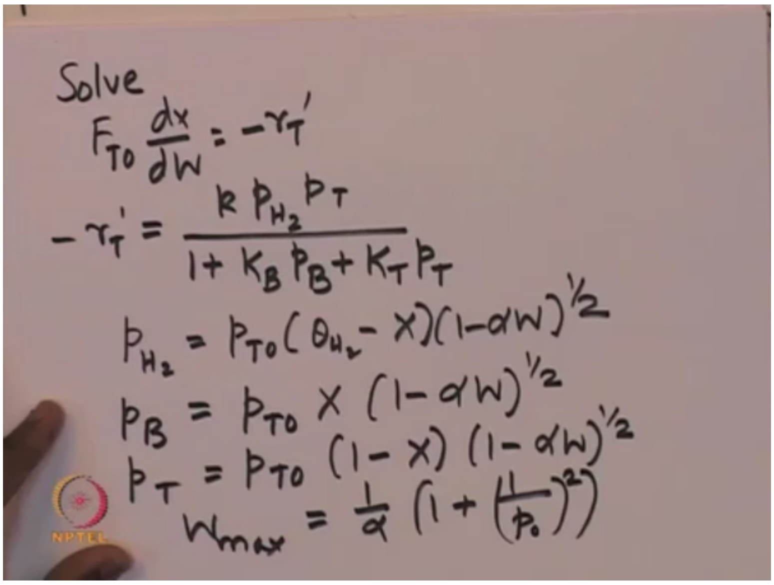

Solve

$$F_{T0}\frac{dx}{dW} = -r_T'$$

$$-r_T' = \frac{k P_{H_2} P_T}{1 + K_B P_B + K_T P_T}$$

$$P_{H_2} = P_{T0}(\theta_{H_2} - x)(1-\alpha W)^{1/2}$$

$$P_B = P_{T0}\, x\, (1-\alpha W)^{1/2}$$

$$P_T = P_{T0}(1-x)(1-\alpha W)^{1/2}$$

$$W_{max} = \frac{1}{\alpha}\left(1 + \left(\frac{1}{P_0}\right)^2\right)$$

So, we need to solve this equation F T nought into d X by d W = – r T prime with the rate of the equation being, rate of the generation of species toluene being k into partial pressure of hydrogen, partial pressure of toluene, divided by 1 + the equilibrium constant for benzene, multiplied by the partial pressure of benzene + the equilibrium constant of toluene multiplied by the partial pressure of toluene.

And we know that partial pressure of hydrogen is = P T nought into theta H 2 – X into 1 – alpha W to the power of half. And then the partial pressure of benzene is given by the inlet partial pressure of toluene, multiplied by the conversion into 1 – alpha W to the power of half. And the partial pressure of toluene is given by P T 0 into 1 – X into 1 – alpha W to the power of half. And the maximum weight of the catalyst is given by 1 by alpha into 1 + 1 by P 0 to the power of 2.

So, this gives you the, this captures the model equations and all the others necessary relationship between the partial pressures and the conversion in order to find the conversion as a function of the weight of the catalyst. So, remember that the weight of the catalyst at the inlet of the reactor is 0 and at the outlet of the reactor is the maximum weight that can be packed, maximum catalyst that can be packed inside the reactor.

So, let us look at how the solution is going to look like. So, if we have the numbers and if we have the quantities, all the required quantities, then in principal we should be able to integrate this expression and find the profile of conversion as a function of weight of the catalyst. So, let me just sketch, here I will sketch the profile of the conversion as a function of weight of the catalyst.

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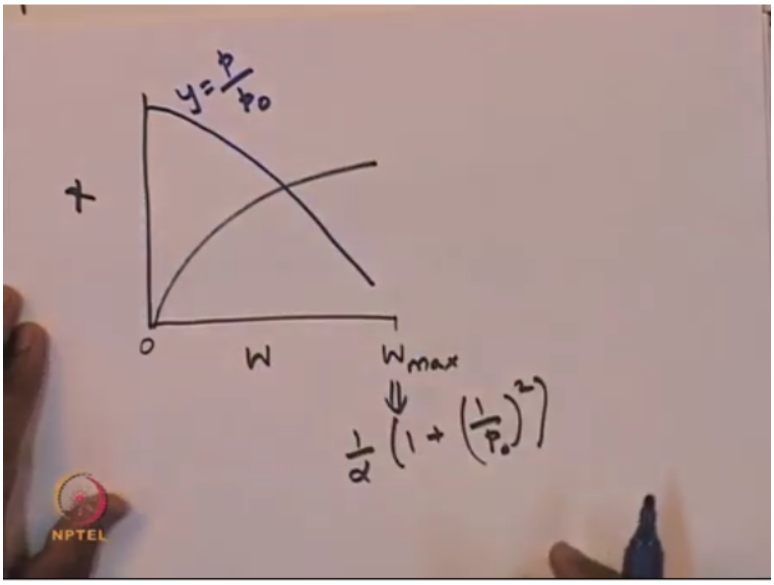

So, suppose in the x-axis I have the weight of the catalyst going from 0 to the maximum weight. So, remember that the maximum weight is given by 1 by alpha into 1 + 1 by P nought the whole square. And if I plot X which is the conversion. Then the conversion as you go into the reactor as the fluid stream sees more catalyst, you see that there is an increase in the conversion as a function of the weight of the catalyst.

While if you look at the pressure drop inside the mole fraction inside the reactor. The mole fraction y, the overall mole fraction y actually goes down. So, this is y = P by P nought. So, that actually goes down because the reaction is being conducted and the reaction is happening as the fluid stream goes through the reactor. We can actually get much more information than this. So, we can actually look at the how the partial pressure changes to the with the weight of the catalyst.

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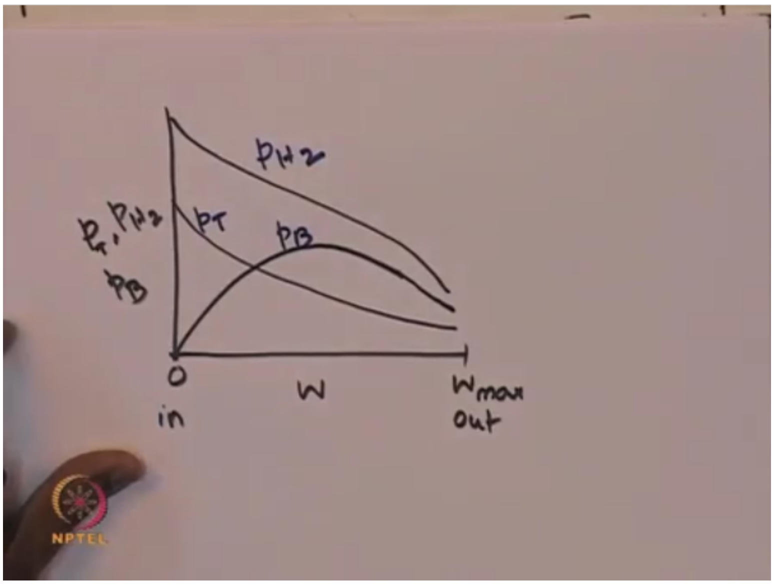

So, if I plot, that is the maximum weight of the catalyst. That is the exit of the reactor. So, this is the inlet stream and this is the outlet stream, that is the outside location of the reactor. And so, if I plot the partial pressures of toluene, partial pressure of hydrogen and partial pressure of benzene for typical set of parameters, we will see that the partial pressure of hydrogen has a profile which looks like this.

And then we have a toluene partial pressure which actually decreases, because toluene is being consumed. And then the benzene partial pressure, this is the kind of profile that is observed. Now, the reason for, so this is for, this is the partial pressure for hydrogen, partial pressure for toluene and the partial pressure of benzene. Now the reason why the partial pressure of benzene goes through a maxima is because we said that the outside pressure is, the pressure of at which the stream leaves the reactor is 1 atmosphere.

And so, there is clearly a pressure drop and there and pressure drop actually causes the partial pressure of benzene to go through a maximum and then towards the exit of the reactor it starts falling down. So, this sort of captures systematically the method for designing a reactor starting from experimental data. So, let us look at a, what happens if the, if we conduct the reaction under fluidised CSTR.

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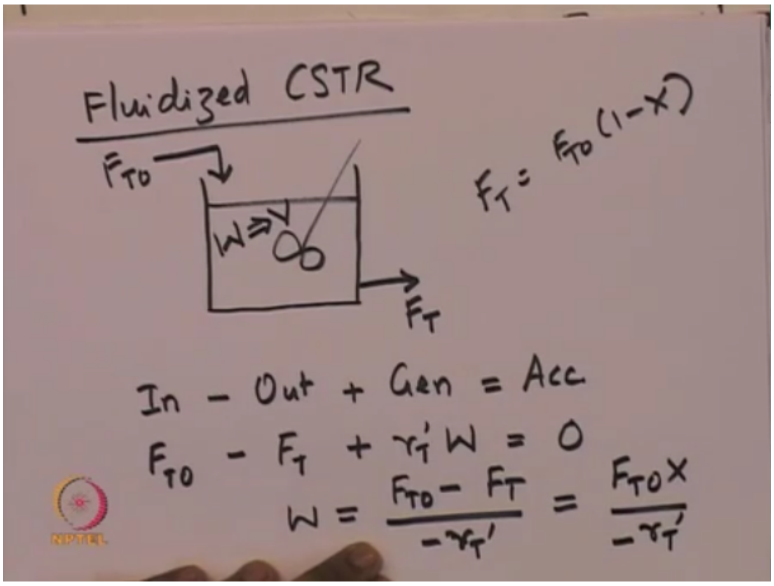

So, suppose if we take a fluidized CSTR. So, CSTR is essentially a tank. And there is a feed that goes into the CSTR. And it is well mixed and there is a fixed volume. And there is an outlet stream. Generally, for a fluidized bed the inlet is at the bottom and exit at the top. Just for sake of convenience, we assumed other way here. So, the question is how much catalyst weight, weight of the catalyst or how much catalyst that needs to be packed, which directly correlates to the volume of the reactor.

So, how much catalyst has to be packed inside the CSTR in order to obtain the same conversion. So, if F T nought is the molar flow rate of toluene, at the inlet stream of the CSTR and F T is the molar flow rate at which the toluene leaves the reactor. Then a simple mass balance can be, mole balance can be written in order to estimate the amount of catalysts which is required for obtaining the same conversion in a fluidized CSTR.

So, the simple mass balance, mole balance is that the rate at which the stream enters the reactor – the rate at which things leave + the generation should be = the accumulation. So now, what, the rate at which moles enter the CSTR is given by F T nought for toluene – the rate at which it leaves is F T + the rate at which it is generated is given by r T prime which is basically the moles of toluene consumed per gram of catalyst per unit time, multiplied by the weight of the catalyst.

And that should be = 0 if it is a steady state. So, we can now rewrite this equation and we can say that the weight of the catalyst is given by F T 0 – F T divided by – r T prime. So, from here we know that F T which is the rate, molar rate at which the, molar flow rate at which the species leaves the reactor is related to the conversion. Because F T is given by F T nought into 1 – X. So, therefore we can rewrite this expression as F T nought into X divided by – r T prime.

So, if we know what is the conversion in the packed bed reactor, then we should be able to use that conversion. And if it is under the same condition, that is the same flow rate, molar flow rate at which the species enters the CSTR, then we will be able to estimate what is the weight at which the same conversion can be obtained if we use a fluidized CSTR. And this provides an important parameter in terms of designing the reactor.