Advanced Chemical Reaction Engineering
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Lecture - 41
Illustrative Example Gas- Solid Reaction RTD Models Reaction Network

We are looking at advanced reaction engineering practice problems in gas solid reactions. This specific application you are looking at is sponge iron technology; of course, the context is very simple. Steel is a very large commodity around the world and blast furnace is the technology which is a commonly engaged, and we all know that blast furnace is a very large capacity kind of technology and investments are very large; footprints are very large; environmental impacts are also significant and so on. And of course, it would cause movement of materials, availability of raw materials and so on.

Now sponge iron is a technology which is a quite suitable for very small scale; therefore, it is able to use over soft local origin and so on. So, it is something that is gaining ground in different parts of the world particularly in India, okay.

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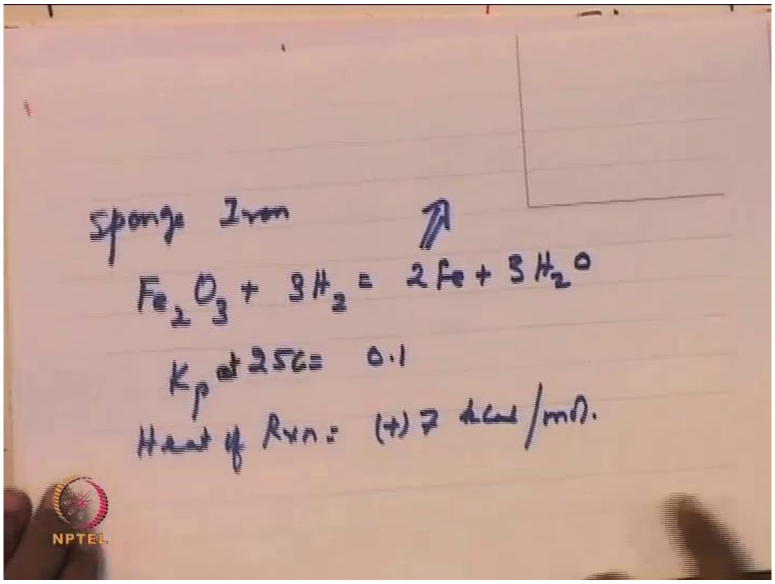

Sponge Iron

$Fe_2O_3 + 3H_2 = 2Fe + 3H_2O$

K_p at 25C = 0.1

Heat of Rxn: (+) 7 kcal/mol.

So, we will look at that very briefly; you have an ore which is iron, iron ore as you can see. It is reacted with gas hydrogen to form iron and water. So, this is the reaction. The equilibrium constant at 25 c is 0.1 showing that you know it is an endothermic reaction. So, you need high temperatures to reach reasonable velocities reasonably favorable equilibrium constants and so on.

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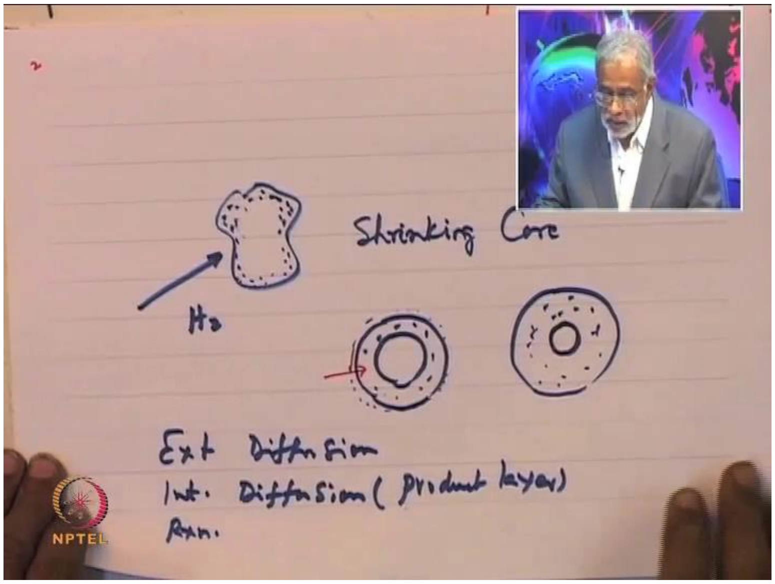

But if you look at a reaction a particle I mean generally particles are at various sizes never spherical but enough in the point of view of doing analysis. We assume that it is a spherical particle, and this particle will react; there is an external diffusion as you can see there is a resistance in external layer as the gas moves through, okay. So, there is an external diffusion resistance; there is an internal diffusion resistance, the resistance to the flow of gas, movement of gas through the product layer.

As the reaction proceeds, the product layer keeps on becoming bigger and bigger; therefore, this resistance becomes larger and larger as the reaction proceeds plus the reaction takes place at the interface here let us say and there is a resistance due to reaction. I mean this is a very simplistic model of what might be happening. What happens is much more involved than what I am saying; therefore, there are three types of resistances that are important for a reaction of this nature, okay.

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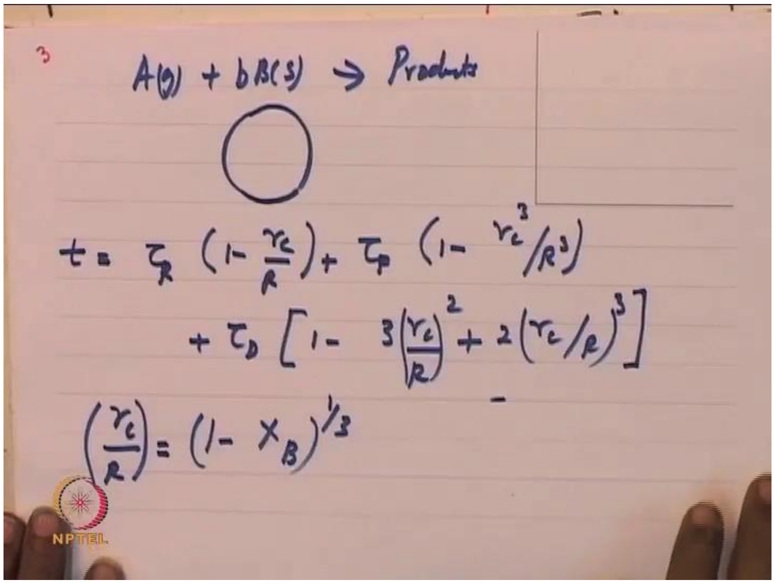

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$$A(g) + bB(s) \rightarrow \text{Products}$$

$$t = \tau_R \left(1 - \frac{r_c}{R}\right) + \tau_P \left(1 - r_c^3/R^3\right) + \tau_D \left[1 - 3\left(\frac{r_c}{R}\right)^2 + 2\left(r_c/R\right)^3\right]$$

$$\left(\frac{r_c}{R}\right) = (1 - X_B)^{1/3}$$

We have at an earlier stage looked at problems like this and we have formulated this a gas plus b b solid giving products a reaction of this form. In this case, for example, in our case you have a gas. So, this is gas; so this is a b b solid. Let us say b b solid, so giving you products. The two products are given here. So, a gas will be b solids and giving you product; we are looking at and then the idealized form of this is what we are looking at and we have at an earlier stage if you recall in the course, we have shown that the time required for this reaction to undergo a certain extent of reaction. Let us say if x b is the extent of reaction, okay, which is r c by r, then given x b you can find out the time that is required for this extent of reaction.

So, this we have already formulated and derived at an earlier stage; we will not do it again. What is important to recognize here that there is a reaction time, there is an external diffusion time and there is an internal diffusion time; all three of them together determine the actual time that is taken for the reaction to occur, okay. Now we also recognize that all these resistances all these we have shown this earlier in our classes and then we are just using those results at the moment.

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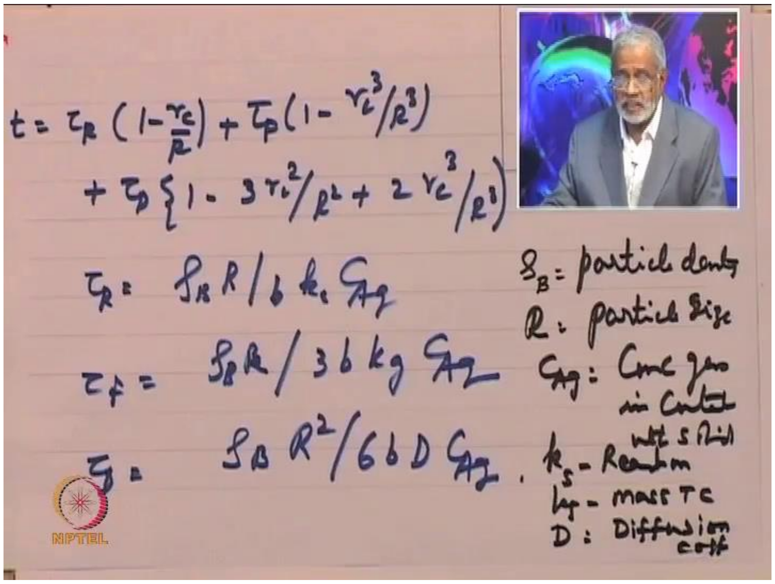

$$t = \tau_R \left(1 - \frac{r_c}{R}\right) + \tau_F \left(1 - r_c^3/R^3\right) + \tau_D \left\{1 - 3 r_c^2/R^2 + 2 r_c^3/R^3\right\}$$

$$\tau_R = \rho_B R / b k_s C_{Ag}$$

$$\tau_F = \rho_B R / 3 b k_g C_{Ag}$$

$$\tau_D = \rho_B R^2 / 6 b D C_{Ag}$$

ρ_B = particle density

R : particle size

C_{Ag} : Conc gas in contact with solid

k_s - Reaction

k_g - mass TC

D : Diffusion coeff

So, you have the total reaction time which is sum of the reaction time due to individual resistances where the reaction time for time for complete consumption if it is a reaction control, film diffusion control or product layer diffusion control; these are all also derived in class. Just to contextualize what we are saying rho b is the particle density. This rho b is particle density, okay. You have r is particle seize, okay, then this is c a g is concentration gas in contact with solid, okay, alright. Now the way the formulation has been done is that the gas concentrations have been assumed to be so large that it does not change during the course of reaction. That is an example that we have taken but we will try to relax all this as we go along, okay.

Now k s is reaction velocity, okay; k g is mass transfer coefficient, okay and then d is diffusion coefficient or internal diffusion coefficient. So, what we are here is that the time required for consumption of the particle is determined by all three factors, the reaction, external diffusion resistance and internal diffusion resistance, okay. So, we can do a small calculation just to get a feel for the kind of numbers we will get in the case of what we call as sponge iron. So, I have got some numbers here; let me just put down those numbers.

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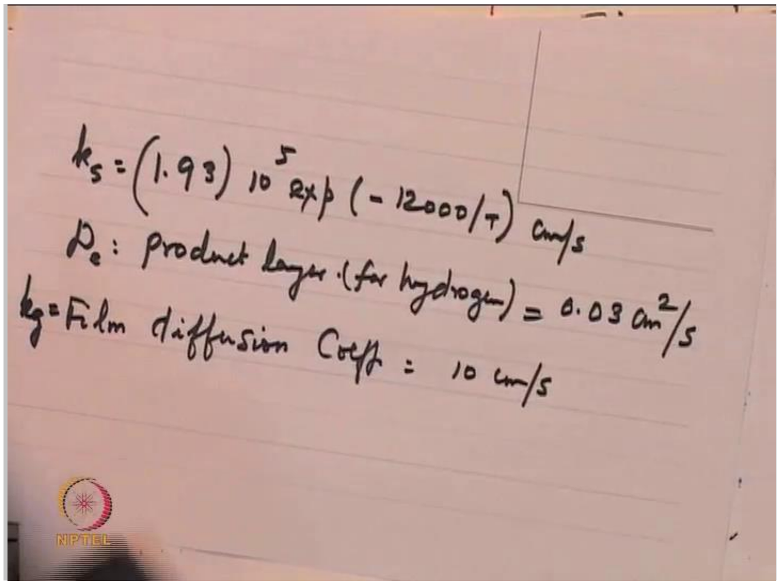

$k_s = (1.93)\, 10^5 \exp(-12000/T)$ cm/s

D_e : Product layer (for hydrogen) $= 0.03\ cm^2/s$

k_g = Film diffusion Coeff : 10 cm/s

You have k s equal to 1.93 10 rise to power 5 exponential of minus 12000 by t. This is in centimeters per second, then diffusion coefficient d in product layer; that means hydrogen diffusion coefficient, this is for hydrogen, okay. This data is given as 0.03 centimeter square per second; this is given. Film diffusion coefficient film diffusion equal to 10 centimeters per second; these are all data given to us. So, recall that the time required depends upon tau r tau f and tau d, and tau r tau f tau d depends upon the concentration of gas which you will calculate shortly and, of course, k s, k g and diffusion coefficient.

So, basically this data is given to us; we have to do some calculation to find out what is the actual time that is required, okay; that is the point. So, this is k g, okay. So, let us do these calculations and then find out what is actual time that is required for this reaction, okay. Let me just do a small calculation for you.

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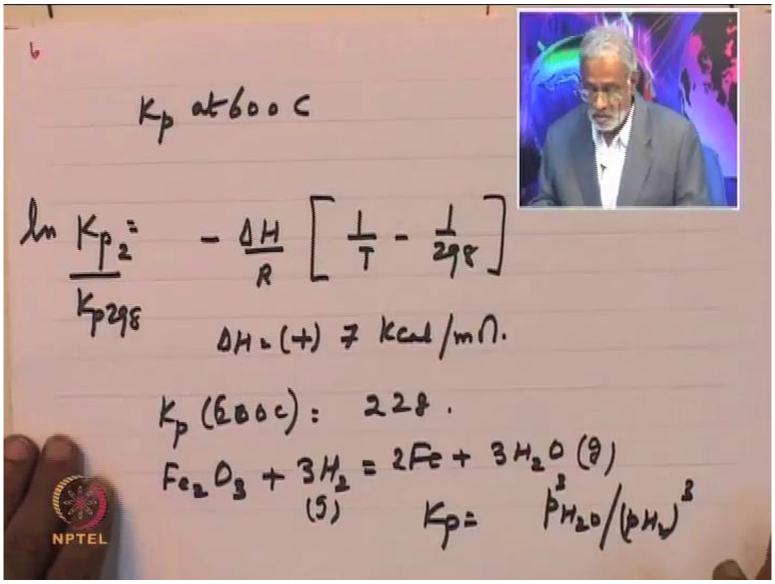

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K_p at 600 C

$$\ln \frac{K_{p_2}}{K_{p298}} = -\frac{\Delta H}{R}\left[\frac{1}{T} - \frac{1}{298}\right]$$

$\Delta H = (+)\ 7$ Kcal/mol.

K_p (600 c) : 228.

$Fe_2O_3 + \underset{(g)}{3H_2} = 2Fe + 3H_2O\ (g)$

$K_p = p^3_{H_2O}/(pH_2)^3$

What is k p? K p we know this l n at say two we will say at k p at 298 and our reactions are taking place at 600 c; we want to k p at 600 c, okay. So, we want this. This we know is delta h by r; this is van’t Hoff equation. So, we know all this. So, you can put your numbers; delta h is given as plus 7 kilo cal per mole, this is given. So, you put all these numbers. So, k p at 600 c comes out to be 228. So, please put the numbers and you will see for yourself, okay; this is 228. Showing that in this temperature, the reaction is quite favorable. Now our reaction is what Fe 2 O 3 plus 3 H 2 equal to twice Fe plus 3 H 2 O, okay. This is gas; this is also gas. So, k p can be put as pH 2 O to the power of 3 divided by p H 2 to the power of 3; this is something that we know from our basic physical chemistry. So, this is nothing new, okay.

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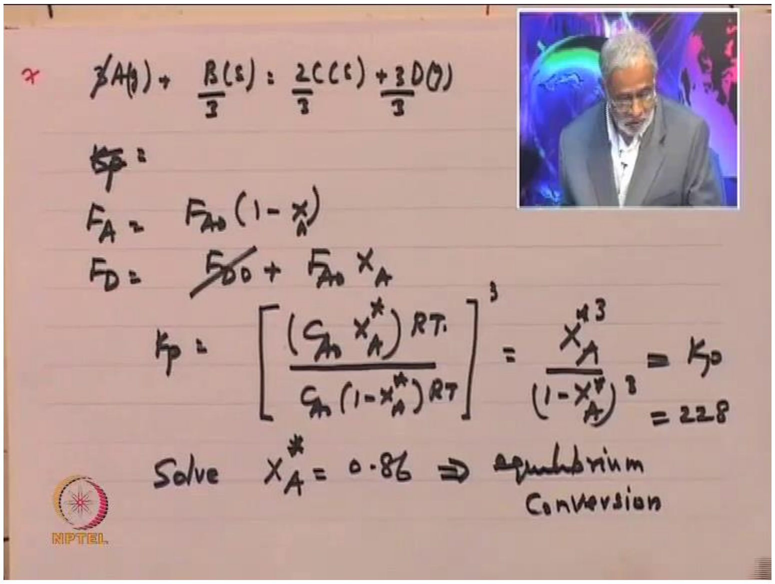

$$\cancel{3}A(g) + \frac{B(s)}{3} = \frac{2C(s)}{3} + \frac{3D(g)}{3}$$

$$\cancel{K_p} =$$

$$F_A = F_{A0}(1 - x_A)$$

$$F_D = \cancel{F_{D0}} + F_{A0} x_A$$

$$K_p = \left[\frac{(C_{A0} x_A^*) RT}{C_{A0}(1 - x_A^*) RT}\right]^3 = \frac{x_A^{*3}}{(1 - x_A^*)^3} = K_p = 228$$

Solve $x_A^* = 0.86 \Rightarrow$ equilibrium conversion

Now let us go through the whole exercise one by one. Now k p equal to so if you look at this reaction, if this reaction is a gas plus b solid giving you c solid plus d gas, okay. So, I can this there is a three here which you can divide. So, it becomes 1 by 3 and then this is 2 by 3 and there is a 3 here by 3, okay. So, we can look at our stoichiometry; f a become f a 0 times 1 minus of x, we know this, okay. This is gas, okay, and then f d equal to f d 0 which is given; it is not given. So, we take it as 0 f a 0 x a I will put it x a; therefore, k p we write as c a 0 x a. We can put an r t here, okay, divided by c a 0 times 1 minus of x a to an r t here to the power 3.

That is equal to x a to the power of 3 divided by 1 minus of x a to the power of 3, okay; this is equal to k p. So, we can solve this k p is given as 228. So, we have this is equal to 228 is given, okay, solve; how do we solve this? Take the cube of 228; let me just see if we have to calculate or I do not have here right now. So, solve we can take cube root of 228 and then find x a to be solved and x a comes out to be 0.86, okay. It is valid the elementary you take cube root of 228 straightaway we will get the answers, okay, alright.

So, since it is equilibrium I am putting star here; I am putting a star here, putting a star here, putting a star here showing that this is the equilibrium conversion. This is the equilibrium conversion possible, okay. This is implies equilibrium conversion, okay. Now clearly we will practice; we do not reach this. We can only approach this, okay. Let us go further, you know x a star. Now we have gone through all that exercise and so on. So, let us not spend too much time; we have shown see our x the problem that we are trying to solve is you have 2 mm particle.

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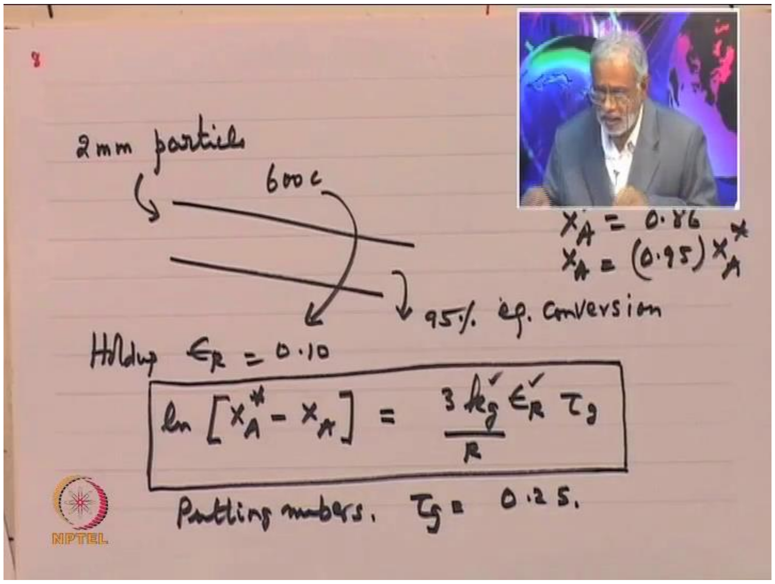

2mm particle

600 c

95% eq. conversion

$x_A = 0.86$

$x_A = (0.95)\, x_A^*$

Holdup $\epsilon_R = 0.10$

$$\boxed{\ln\left[x_A^* - x_A\right] = \frac{3 k_g \epsilon_R}{R} \tau_g}$$

Putting numbers. $\tau_g = 0.25$.

It says 2 mm particle, okay, and it is a rotary kill, okay; there is a rotary kill which is rotating, okay, which is rotating. Solids are coming in; solids are coming down, okay. So, you want here 95 percent equilibrium conversion; this is the problem statement. 600 c is the temperature of the kill. Now the hold up here epsilon r hold up of solids is 0.1, okay; that is also given. Now we have gone through all the exercise; we have set of equations before. So, there is no need to do the exercise again. So, we know that this is given as l n; we now this. So, I am just writing the final form l n of x a star by minus of x a; we know this, okay, equal to k g epsilon r three times divided by r tau g.

So, this is a result that we have gotten much earlier. So, I am just putting that result right now. So, this is something that we know, okay. Now all the numbers are given here, okay. So, you can put all the numbers and then find out tau g. So, when are you putting numbers, I am just putting numbers. What are the numbers here? X a star is given as 0.86, and x a is given as 0.95 of x a star. So, you know x a star, you know x a; k g is given, okay and then epsilon r is 0.1. The size of the particle is 2 millimeter that is also given; putting all the numbers, I will find that tau g comes out to be 0.2 seconds, okay. So, essentially what we are saying is that the gas residence time is quite small, okay. So, gas residence times are quite small, okay.

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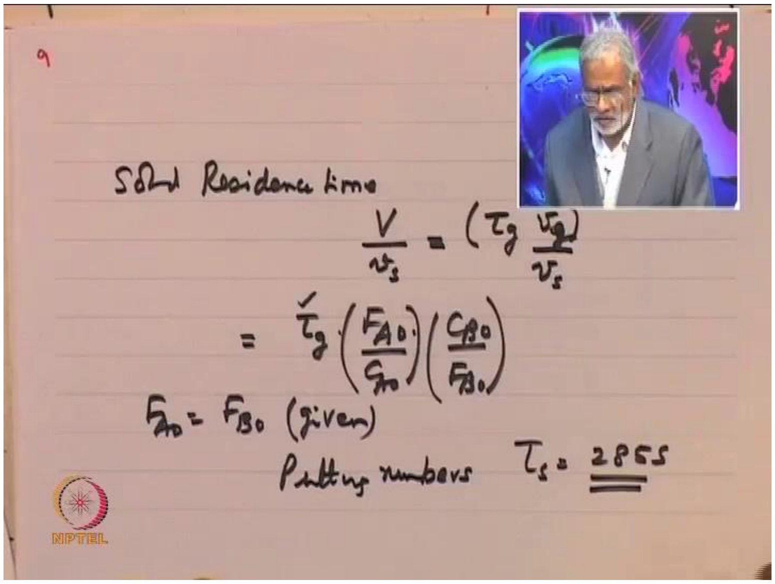

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Solid Residence time

$$\frac{V}{v_s} = \left(\tau_g \frac{v_g}{v_s}\right)$$

$$= \tau_g \left(\frac{F_{A0}}{C_{A0}}\right)\left(\frac{C_{B0}}{F_{B0}}\right)$$

$F_{A0} = F_{B0}$ (given)

Putting numbers $\tau_s = 285 s$

Now what we want is solids residence time. So, how do you relate gas residence time to solid's residence time? Solid's residence time is what by definition it is volume of equipment divided by the solid's flow, correct. From our stoichiometry, we know it is tau g v g by v s, okay; volume of the equipment is gas residence time minus the gas flow divided by v s, okay. Now that is equal to tau g and then sorry v g. What is v g? V g is f a 0 by c a 0, okay, and then c b 0 by f b 0, is that clear. So, what is given? F a 0 is given as equal to f b 0 is given, okay; this data is given, okay. So, that if you put all these numbers now putting numbers f a 0 is okay.

So, you get this f a 0 equal to f; they cancel off, c a 0 and c b 0 put all the numbers. It turns out that tau s equal to 285 seconds, okay; how do you get this? Tau g is given; we have got in the previous case c a zero, c b zero, all the data is given. So, what are we trying to say? That if you have a rotary kill context once again let us not forget. Context is that we have a rotary kill, particles are coming in and hydrogen is fed like this, okay; it is hydrogen and this is iron ore, okay and then what you get here is f e and this moisture escapes, is it okay. So, we are able to tell what is the kind of size of equipment that is required for your application. We have already done we have not yet finished what is called; suppose we do this same process in the laboratory that part we have still not done. Let us do it quickly, so that we can find out what is the time required for.

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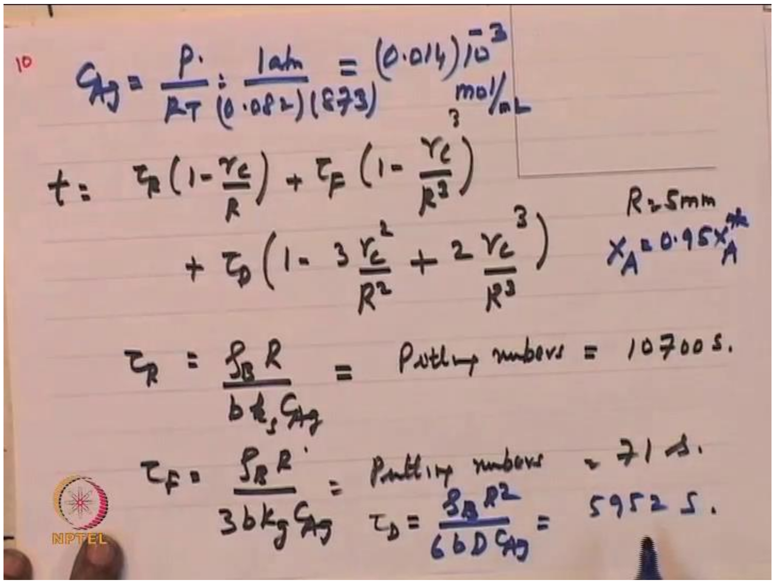

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$$C_{Ag} = \frac{p}{RT} = \frac{1\,atm}{(0.082)(873)} = (0.014)10^{-3}\ mol/mL$$

$$t = \tau_R\left(1 - \frac{r_c}{R}\right) + \tau_F\left(1 - \frac{r_c^3}{R^3}\right) + \tau_D\left(1 - 3\frac{r_c^2}{R^2} + 2\frac{r_c^3}{R^3}\right)$$

$R = 5mm$

$X_A = 0.95 X_A$

$$\tau_R = \frac{\rho_B R}{b k_s C_{Ag}} = \text{Putting numbers} = 10700\,s.$$

$$\tau_F = \frac{\rho_B R}{3 b k_g C_{Ag}} = \text{Putting numbers} = 71\,s.$$

$$\tau_D = \frac{\rho_B R^2}{6 b D C_{Ag}} = 5952\,s.$$

So, we said total time is equal to tau r into 1 minus of r c by r, okay, plus tau f 1 minus of r c cube by r cube, then we said tau d equal to 1 minus thrice r c squared by r squared plus twice r c cube by r cube, okay. Now so all these we know tau r equal to rho b r divided by b k s c a g rho f equal to rho b r divided by thrice b k g c a g, okay. Now this particular case what is given is that the size of the particle is given as what 5 millimeter size. So, particle size r is given as 5 mm, okay, and then k b all these k s and all that it is given; putting numbers we get tau r equal to tau r turns out to be about 10700 seconds putting numbers.

Similarly, putting numbers here putting numbers, we get tau f turns out to be 71 seconds, okay, and similarly, tau d I will write here tau d equal to rho b r squared. Let me write here rho b r squared divided by 6 b d c a g; putting numbers it comes out to be how much 5952, okay, seconds. Now c a g I did not calculate c a g is p by r t, okay, that turns out to be p by r t, okay. P is one atmosphere; r is 0.082, okay, and t is 600 and 273 is about 873. So, that turns out to be 0.014 10 minus 3 mole per milliliter, okay.

So, basically what I am trying to put across to you is that we can now calculate. Since, you know tau r, tau f and tau d, we can now calculate what is t. So, what is the question that is asked is the question that is 95 percent of equilibrium conversion. So, you have been asked to find x a which is equal to 0.95 times x a star; we have got x a star already, okay. Lets us just do that calculation; it is an important calculation.

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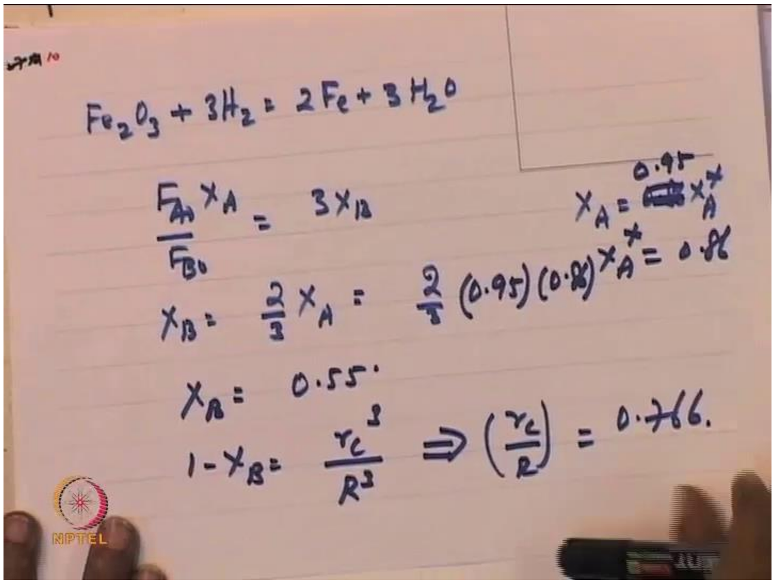

$Fe_2O_3 + 3H_2 = 2Fe + 3H_2O$

$\frac{F_{A0} X_A}{F_{B0}} = 3X_B$

$X_A = 0.95\, X_A^*$

$X_B = \frac{2}{3} X_A = \frac{2}{3}(0.95)(0.86)$

$X_A^* = 0.86$

$X_B = 0.55.$

$1 - X_B = \frac{r_c^3}{R^3} \Rightarrow \left(\frac{r_c}{R}\right) = 0.766.$

Let us just do that. Our reaction is Fe 2 O 3 plus three hydrogen equal to twice Fe plus three H 2 O, okay. Now f a 0 x a h a by f b 0 equal to thrice x b. So, x b equal to 2 by 3 x a, okay; that is 2 by 3 of x a, what is x a? We have got x, we have got x a as 0.86 times x a star, okay, 0.86 x a star. So, we can put all these things; x a star is we have already derived that x a star is point sorry x a is equal to 0.95 x a star sorry. And x a star is 0.86. So, we can put all these things 0.95 multiplied by 0.86. So, that comes x b comes out to be 0.55, okay.

Now 1 minus of x b by definition is r c cube by r cubed, okay. So, x b is known; this implies r c by r equal to 0.7 double six, okay, is that clear. Now once you know x r c by r, now we can calculate once you know r c by r we go back. Now our expressions are as are all here so r c by r for our application is i will just write here just for sake; for sake of simplicity r c by r becomes 0.766. Once you put r c by r values here you should be able to find what is the time for complete for the extent of reaction desired. So, what in essence we are saying is that the time required for our case. So, the time required is if you put all these numbers, the time required comes out to be something like this.

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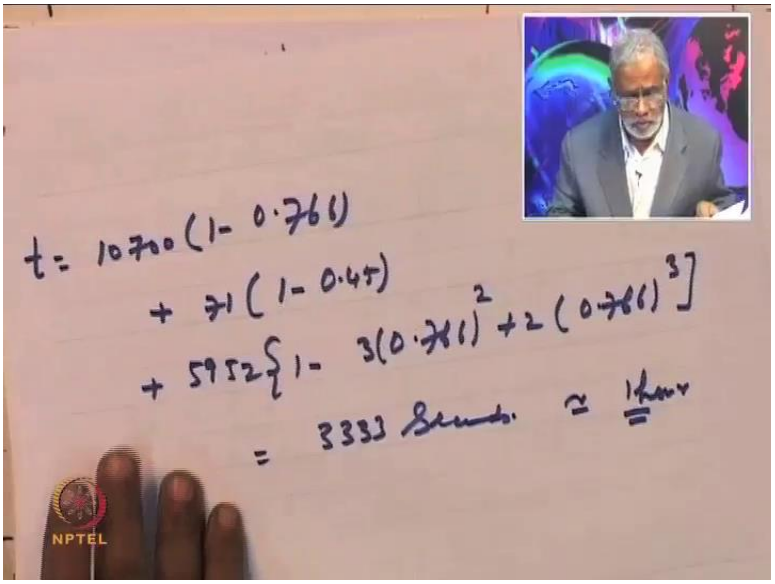

$$\begin{aligned} t = {} & 10700(1-0.761) \\ & + 71(1-0.45) \\ & + 5952\{1-3(0.761)^2+2(0.761)^3] \\ = {} & 3333\ \text{Seconds} \simeq \underline{\underline{1\,\text{hour}}} \end{aligned}$$

Let me write down t equal to 10700 multiplied by 1 minus of 0.766 plus 71 one minus of 0.766 whole cubed is 0.4, okay, plus 5952 one minus three times 0.766 whole squared plus two times 0.766 whole cube, okay. So, when we need to do all this, it comes out to be 3333 seconds, okay. So, it is close to approximately 1 hour. So, what we are saying is that see in this exercise, what we are trying to do is the following that we have looked at a problem which is of commercial interest which is of considerable interest because small scale industries are important and then its where we make what we sponge iron; see we are making sponge iron.

So, what we are trying to calculate here is that what is the time that may be required to get a certain extent of reaction, okay. If you do an experiment in the batch equipment but what we also pointed out is that when we do this experiment or do this in a rotary kill; when it is in the rotary kill, what we find is that because of the rotation of the kill, the external surface gets sheared off. The product layer gets sheared off and to an extent and more importantly if sheering of may not be all that good but more importantly because of the fact that lot of gases are coming out, and then it is quite porous.

And as a result, those resistances may not be significant I mean nor that is the kind of assumption we have made in this calculation; I mean in reality these mean may not be correct. This resistance will have to take into account and so on. So, what we are trying to do here is that if we can manufacture sponge iron using a technology like this in a rotary kill, where it gives you continuous productions and so on. And then you have to, of course, ensure that the temperatures are managed and then heat losses are minimized and so on, okay. So, this example illustrates how we can use the procedures that we have developed during the course of last several months and how we can apply them to understand a fairly important commercial process, okay.

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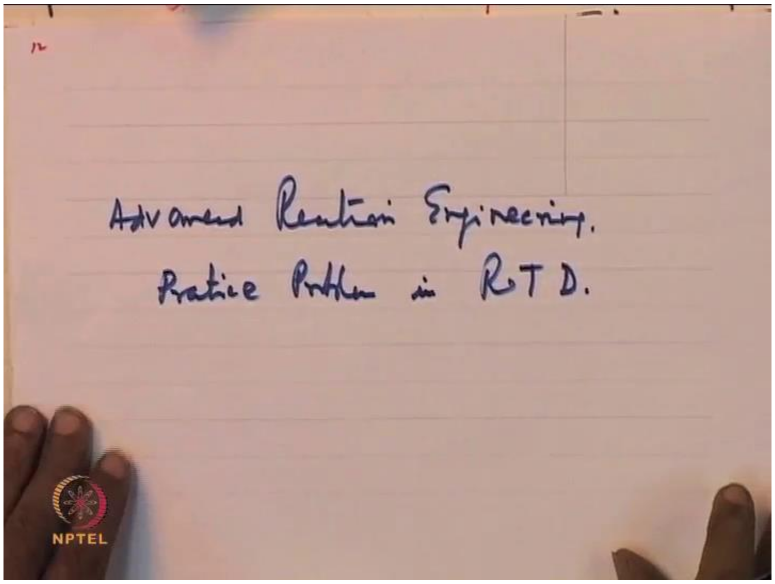

Advanced Reaction Engineering.

Pratice Problem in RTD.

Now we will go on to another application. Now we are going to look at what we call as a practice looking at advance reaction engineering once again, okay. Now the application we are looking at is practice problem in residence time; we call it RTD, okay. So, you have to take an example of RTD; let us see how we can make use of this. Now the example in front of us is the following. It says I mean problem reads like this.

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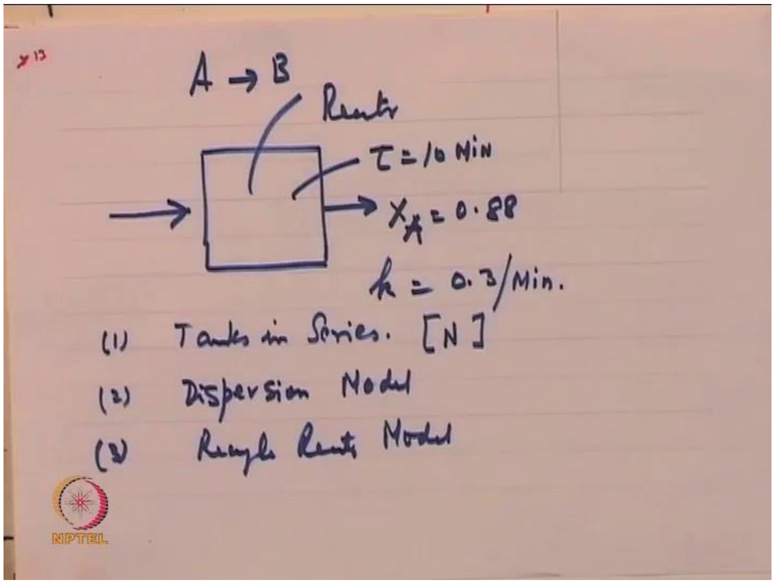

(1) Tanks in Series. [N]
(2) Dispersion Model
(3) Recycle Reactor Model

There is an arbitrary vessel, okay, to which this is a reactor, okay. Now in this reactor you are getting a conversion of x a equal to 0.88; it is given. So, reaction is a goes to b; this is the reaction. Now it says that this residence time here is ten minutes; that is also given. Now the rate constant this rate constant k is given as 0.3 per minute; the rate constant is 0.3 per minute. So, it is modeled as tanks in series, okay, tanks in series. Two, it is modeled as dispersion model. Third, it is modeled as a recycle reactor model. What is being said is when you model an arbitrary vessel as assuming that it can be described as tanks in series, your parameter is n number of tanks.

So, the question that is in front of us is that it is an arbitrary vessel which gives you a conversion of 0.88 for a residence time of ten minutes rate constant 0.3. Now if you modulate as tanks in series model, how many tanks will be required; this is the question, okay. Now if you modulate as a dispersion model, what would be the Peclet number that would be able to describe this experimental data? Now third thing if you describe it as a recycle reactor, what will be the recycle ratio that will be able to capture this experimental result? On other words, what in essence we are trying to do here is that in arbitrary equipment, we may have designed it as a plug flow reactor and so on, but the fact is that it behaves in a certain way; we do not know what the behavior is.

And we have models which is able to account for deviations from idle behavior. This is what we have been doing when we talk about non-ideal reactors; how does it deviate from idle behavior for which we have these models, okay. So, let us do one by one; let us do this one by one. Let us see how what kind of answers we can think off. Now let us look at the simplest and then go on to the more complicated; first, we will see how our system can be described as tanks in series model.

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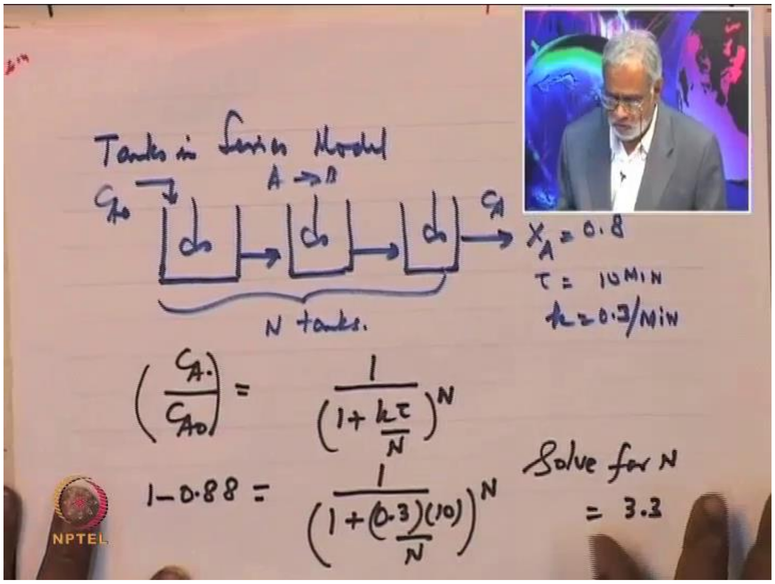

Tanks in Series Model

$A \rightarrow B$

$X_A = 0.8$

$\tau = 10\,MIN$

$k = 0.3/MIN$

$$\left(\frac{C_A}{C_{A0}}\right) = \frac{1}{\left(1+\frac{k\tau}{N}\right)^N}$$

$$1-0.88 = \frac{1}{\left(1+\frac{(0.3)(10)}{N}\right)^N}$$

Solve for N

$= 3.3$

So, what are tanks in series model? Let us just understand what are tanks in series model; what is tanks in series model? Tanks in series model essentially says that our arbitrary vessels can be represented as a number of stirred tanks, okay, and therefore, whatever we get here at the end of these tanks. So, here in this particular case this x a is 0.88, and the total residence time tau is how many minutes? Ten minutes is it, ten minutes, yeah, ten minutes and the rate constant is given as 0.3 per minute, okay. So, this reaction a goes to b is taking place in this equipment; of course, it is broken up as three stirred tanks or four stirred tanks but the fact remains that it is single equipment which is being modeled this way, okay.

Now we know if this is c a 0, okay, if this is c a and let us say this is n tanks in between assuming that there are n tanks, okay. The result says that c a we know this from our experiment; c a by c a 0 equal to 1 by 1 plus k tau by n to the power of n; this result we know, okay. This is a result that we know from our understanding of stirred tanks. Now what is ca by c a 0? It is 1 minus of 0.88, you know this is okay 1 by 1 plus k is 0.3; tau is 10. It is given; what is not known is this n, okay, solve for n. So, when we solve, we find n becomes 3.3. So, I mean you might say how can we have 3.3 number of tanks; I think that is not the issue. The point is you have an arbitrary vessel, okay; this arbitrary vessel performs in a certain way.

Now how do you try to describe this arbitrary vessel in terms of models that you have; therefore, whenever we are looking at these models, you should recognize that this n is only a parameter. It is a model parameter; it could take any value depending upon the situation. Therefore, n equal to 3.3 only means that here is an instance of an equipment which performs similar to number of tanks between three and four; that is what is to be understood, okay, alright.

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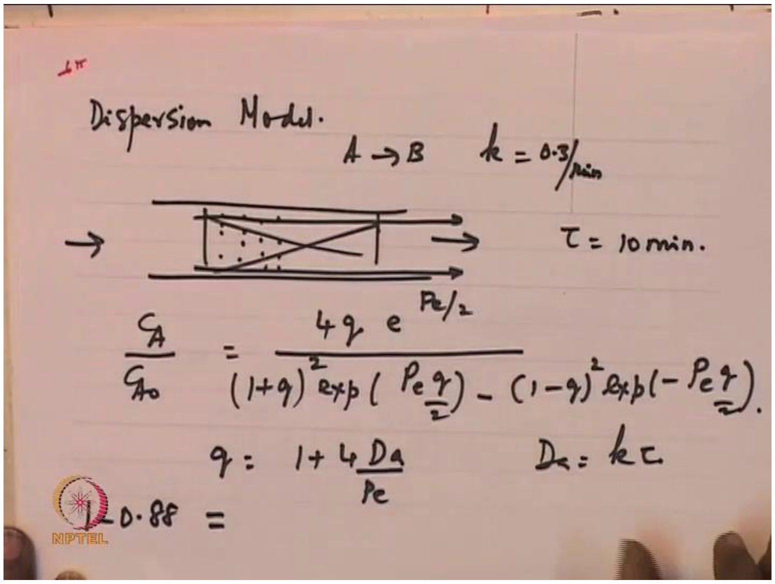

Dispersion Model.

$A \rightarrow B \quad k = 0.3/\text{min}$

$\tau = 10\ \text{min.}$

$$\frac{C_A}{C_{A0}} = \frac{4q\, e^{Pe/2}}{(1+q)^2 \exp\left(\frac{Pe\, q}{2}\right) - (1-q)^2 \exp\left(-\frac{Pe\, q}{2}\right)}.$$

$q = 1 + 4\frac{Da}{Pe} \qquad Da = k\tau$

$1 - 0.88 =$

Now let us take the next example which is instead of tanks in series model, we have dispersion model; what is dispersion model? What we said is that suppose there is a fluid flowing through let us say there is a packing here, okay. Now what we said is that fluids a plug flow means what? Every fluid moves together; they move together; they move together move together. That means fluid elements which are at this level and a fluid element at this level, they move through without recognizing the existence of each other; that is an instance of plug flow, but when there is dispersion what happens is some fluid elements move faster than the other, okay because of dispersions, they are moving faster than the other.

Therefore, the kind of time of residence that fluid elements spend inside the equipment is different from what we might think and the basis of the plug flow model in which all the fluid elements have the same amount of residence time. So, this effect we had taken into account and then we have derived in our equations a certain equation that tells us that suppose this reaction a goes to b and then the rate constant is k first order rate constant k, we have shown this; I am just righting the final result. There is no point in deriving it here, okay, by two divided by one plus q square exponential of p e q by two one minus q whole square exponential of minus p q by two, okay, where q equal to the time colon number equal to one plus four d a by p e, okay.

Now we have done this in an earlier class and if we have not done this, we do not recall this; you have to just look up some books on action dispersion models, yet it is all derived fairly simple things, okay. Now if you want to find out conversion of the exit of this equipment, essentially what you need to know is that d a equal to what is d a? D a is equal t k times tau, okay. Now in this particular case, k is given as 0.3 per minute, okay; we know this and then your residence time is given as ten minutes, okay. So in this for this equation, the left hand side is 1 minus of 0.88 equal to the right hand side. The unknown quantity on the right hand side is Peclet number; there is nothing else. Only Peclet number is unknown.

Now it might be more complicated to calculate left hand side from the right hand side is easier; the reverse is more complicated. So, you have to do a trial and error, okay; you will have to do one trail to find the answer, okay. Now when you solve so when you put your numbers and solve, okay, you will find.

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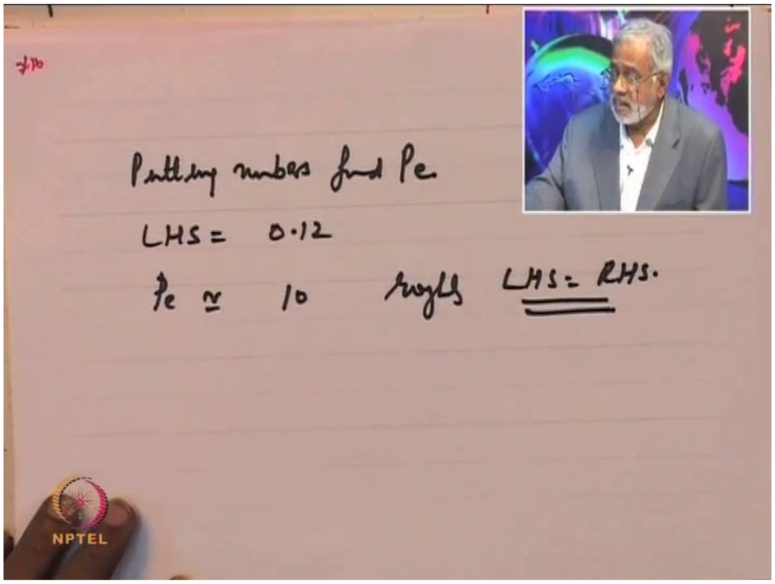

Putting numbers find Pe.

LHS = 0.12

$Pe \simeq 10$ roughly $\underline{\underline{LHS = RHS}}$.

So, putting numbers you can put numbers here is no great problem in putting these numbers, so q putting numbers, okay, find Peclet number corresponding to the left hand side; LHS equal to 0.12. So, Peclet number corresponding to about 10 or so you will find roughly LHS equal to RHS I mean you have to or you can read out these numbers from charts which are available and so on. So, what have we done? What we have done is that we have recognized that you can describe the performance of this arbitrary vessel. This arbitrary vessel conversion here it is 0.88; it is given, okay and then rate constant is given, the residence time is given.

So, what is the parameter Peclet number that would describe this data? The answer is that we should put Peclet number around 10; you will be able to say that the left hand side is roughly equal to right hand side. So, what are we trying to say? What we trying to say is that for this particular instance, the number of tanks equal to 3.3 corresponds to a Peclet number of 10; that is what we trying to say in this particular case, okay, alright. Now there is another way by which we can describe this data; there is another way by which we can describe this data.

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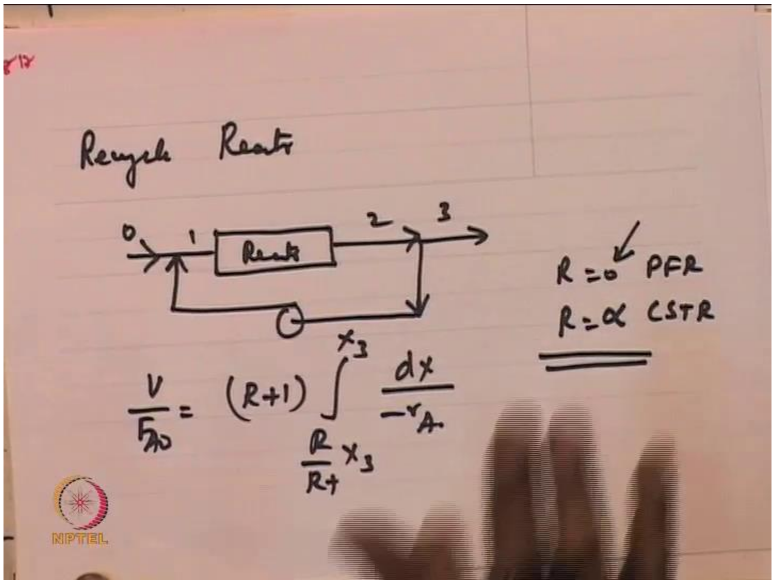

$$\frac{V}{F_{A0}} = (R+1)\int_{\frac{R}{R+1}x_3}^{x_3} \frac{dx}{-r_A}$$

$R = 0$ PFR

$R = \infty$ CSTR

Now if you look at a recycle this is the recycle reactor. Now we said if you recall at an earlier class, we have said that if you have a recycle reactor, okay; this is the reactor, okay. Now depending upon this recycle ratio, the design equation looks like this r by r plus 1; I will call this zero one two and three r by r plus 1 x 3 to x 3 d x by minus of r a. So, when we went through this exercise at an earlier stage, we said that r equal to zero means plug flow PFR; r equal to infinity means CSTR. So, we said at that stage that basically recycle ratio is a way of describing mixing within the equipment.

So, no mixing is r equal to zero; very large amount of mixing is r equal to infinity. And therefore, we can describe various kinds of reaction equipment between no mixing to infinite amount of mixing or PFR to CSTR by adjusting the recycle ratio. We said the same thing when we looked at number of tanks in series. We said when there is one tank two tank and infinite numbers of tanks; we said when there is infinite number of tanks, we are talking about a plug flow reactor. That means n very large means plug flow reactor; n very small means we are having CSTR, okay, n equal to 1 is a CSTR, n equal to infinity is PFR.

So, on another word r equal to 0; that means PFR is equivalent to n equal to infinity, you understand. So, this is what is the kind. So, just like n number of tanks is a way of quantitating the level of mixing; just like Peclet number is a measure of mixing within a reactor, recycle ratio is also a measure of mixing, okay. So, it is a first order reaction; we can integrate this whole thing and the integrated form is available to us. The integrated form I will just write down the integrated form. So, the integrated form for a recycle reaction.

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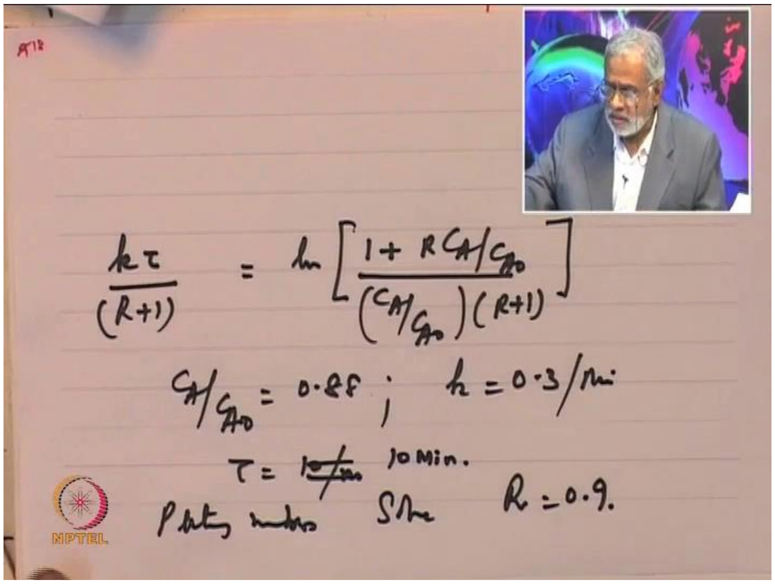

$$\frac{k\tau}{(R+1)} = \ln\left[\frac{1 + R\,C_A/C_{A0}}{(C_A/C_{A0})(R+1)}\right]$$

$C_A/C_{A0} = 0.88$; $k = 0.3/\text{min}$

$\tau = \cancel{10/\text{min}}$ 10 Min.

Putting numbers Solve $R = 0.9$.

So, the integrated form is k times tau divided by r plus 1 equal to ln, within brackets 1 plus r c a by c a naught divided by c a by c a naught multiplied by r plus 1, okay. Now, of course, we can put it in various forms in and so on, but the important thing here is that c a by c a naught is given as 0.88; this is a known, okay. Now k is given as 0.3 per minute and tau is given as 10 minutes. So, putting all these numbers, we can find out value of r. So, solve putting numbers and then solve and then I find that it is around 0.9. When we put so it sort off it satisfies. So, what are we saying? Let us just summarize this; this is an important point what we saying is the following.

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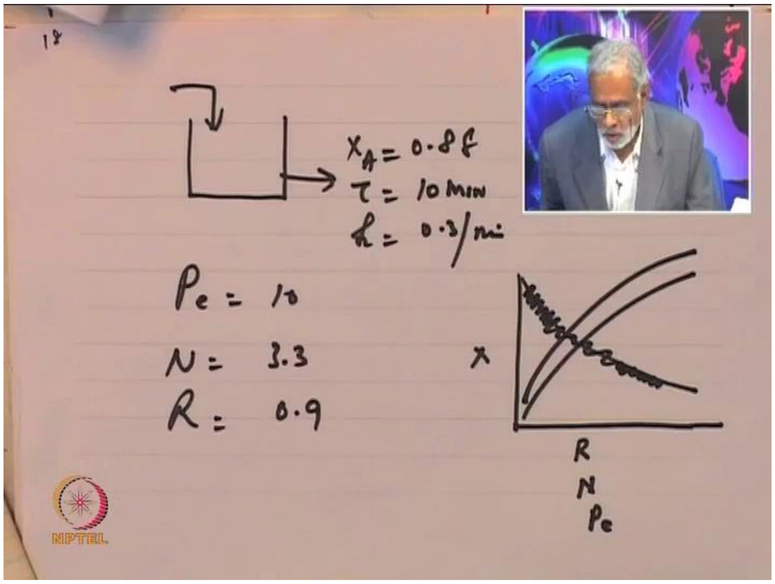

We have looked at an arbitrary vessel, okay; we have looked at an arbitrary vessel. So, we have an arbitrary vessel here coming in and going out, okay. X a is 0.88; tau is 10 minutes; k is 0.3. This are all given; we find Peclet number is put 10, number of tanks is 3.3, recycle ratio is about 0.9, okay. So, what does that mean? What it means is that we are able to see this suppose you make a plot of r versus x, r versus n, r versus p e, okay; I mean we can plot these. So, we can sort of get an idea as r becomes larger and larger, it is CSTR. So, we should expect curves like this, okay.

When n becomes as x that means when r increases, it is going towards, okay; when n is equal to zero, n increases, okay. So, we can plot; on other words what we are trying to say is that as r increases, it is going towards plug flow like this, n increases it is like this and then Peclet number. What do we expect? Peclet number becomes larger and larger and higher the Peclet number, you will have higher is its approach towards a PFR, correct. So, let us understand this one by one. When r becomes large when r becomes let me draw this once again I am not satisfied with this. Let me just do this once again, okay.

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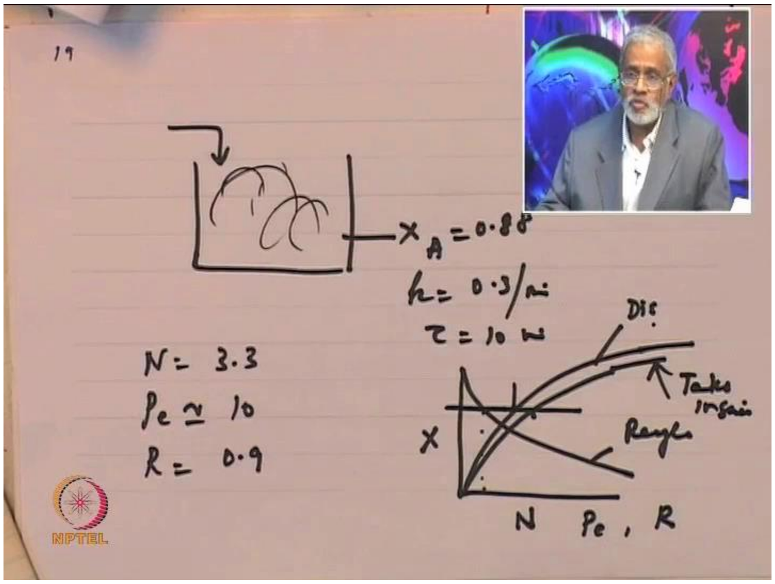

We have a stirred tank; x is 0.88, then k is 0.3 per minute, tau is 10 minutes. Our results are n equal to 3.3; Peclet number is approximately 10; recycle ratio is 0.9, okay. So, all these numbers describes this level of mixing in this equipment, okay. Now we want to understand this in a slightly better way. What we expect? Say suppose, let us say for the same volume if we increase the number of tanks, we will expect that conversion would approach plug flow, okay; that means suppose you have a similarly Peclet number if you draw, you will find that it will approach plug flow, okay. This is what we expect.

Now but you increase r, we will find that it will do this; so this is recycle reactor. This is dispersion model; this is tanks in series model. So, what we are saying is that these are all numbers which can be used to describe a certain level of conversion. Therefore, if our conversion is let us say is 0.88; see if this is 0.88, we can see here these are the numbers we get. This is for dispersion model; this is for tanks in series model; this is for recycle reactor model, okay. So, from this you can tell what are the parameter values for different models? Look at this long story short what we trying to put across in this question. This question essentially says given the data, determine this parameter values which you have done.

Then it says you have to try and understand how these numbers relate to each other. So, this relationship comes out of this; it tells us how conversion changes with the parameter values. So, it gives you qualitative details how these parameters effect extent of reaction, okay. So, this approach to understanding real vessels is very useful when you have an operating process and if you quickly get some data, and you can get from the data what is the kind of mixing that is appropriate to your process. So, it is very useful to get a feel for what is a real life problem. You want to go on to the next exercise an interesting exercise but something that not ready difficult to do.

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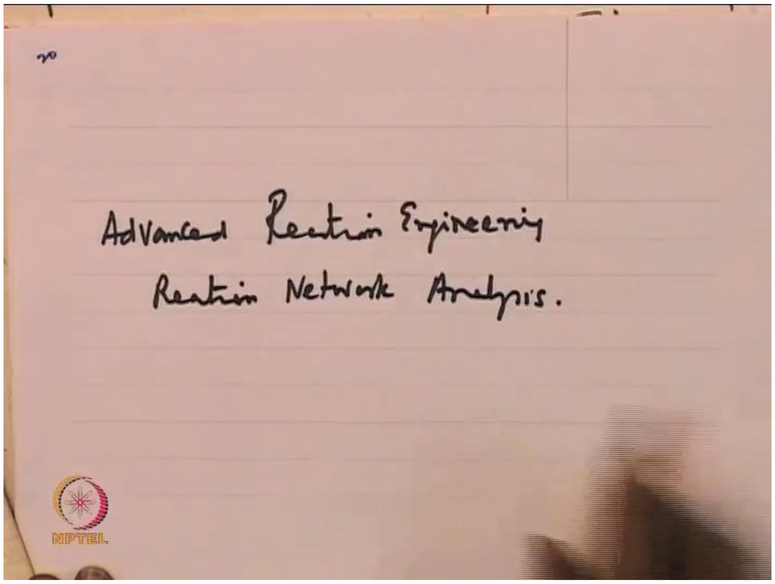

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Advanced Reaction Engineering

Reaction Network Analysis.

So, this exercise we want to do know is advanced reaction engineering, okay; this is let us call reaction network analysis, okay. So, we want to take an example in this reaction network analysis to illustrate how our techniques become so useful in some in many, many instances.

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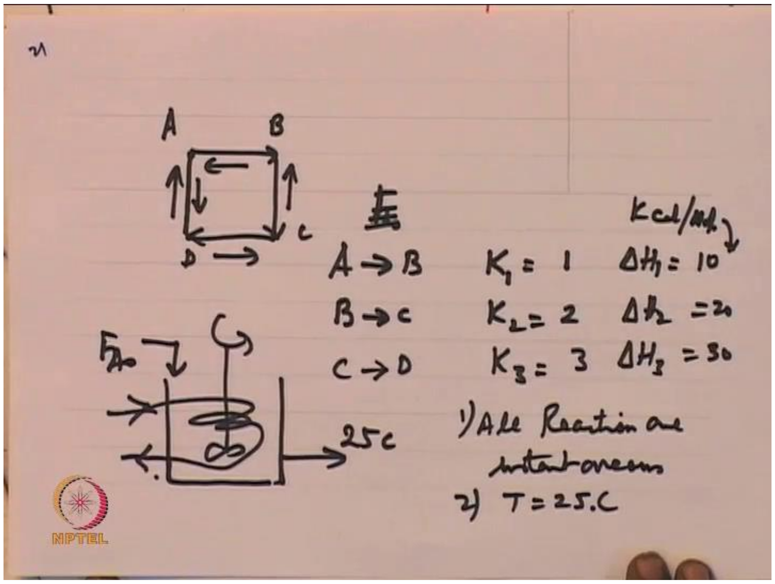

Here is an example of a going to b going to c going to d, okay. So, it is a reaction network; some data is given a goes to b goes to c goes to d a going to b. This equilibrium constant is given as 1; b goes to c b goes to c where are b. K 2 is given as 2; c goes to d k 3 is given as 3. Delta h 1 delta h 2 delta h 3, all these are given. Delta h 1 is 10, 20 and 30; all in units of kilo cal per mole, okay. So, this is the reaction network and this reaction is taking place in a stirred tank, okay. In stirred tank, okay, feed is only pure a is coming going out and then it is a coil to which, which is added. Now the question that is ahead of us is how much heat is to be added or removed; no, that is not the question.

Question is this is operating at 25 c, okay; all these reactions are instantaneous, all reactions are instantaneous, okay. That is one and we are maintaining the temperature at 25, okay. What does it mean to be able to maintain temperature at 2 and there is endothermic reaction is taking place. It implies that we are putting in heat through our heating system. So, here is an instance of continuous input of heat into a reaction system to ensure that these reactions are in there at equilibrium, okay. So, the question in front of us is what is the extent of reaction? So, let me ask this question to you once again; what is the extent of reaction that we should anticipate.

So, what is the extent of reaction we should anticipate when we maintain a temperature of 25 where the reactions a b c d are instantaneous which means that at 25 c, they all exist in their equilibrium, okay, is that clear. So, we have setup this stoichiometry long back. So, there is nothing new for all of you.

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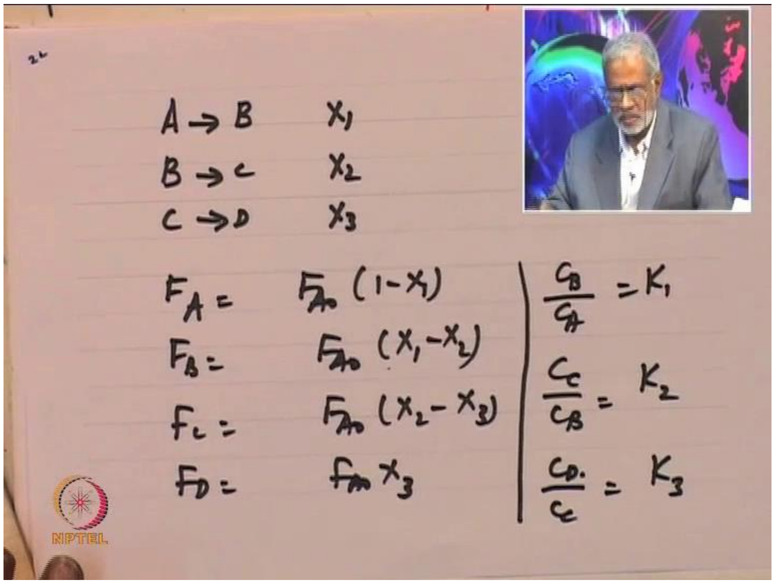

$A \rightarrow B \quad x_1$

$B \rightarrow C \quad x_2$

$C \rightarrow D \quad x_3$

$F_A = F_{A0}(1 - x_1)$

$F_B = F_{A0}(x_1 - x_2)$

$F_C = F_{A0}(x_2 - x_3)$

$F_D = F_{A0}\, x_3$

$\frac{C_B}{C_A} = K_1$

$\frac{C_C}{C_B} = K_2$

$\frac{C_D}{C_C} = K_3$

But just to for the sake of completion I can say; if I say this is x 1, this is x 2, this is x 3 and then our stoichiometry says that f a equal to f a 0 times 1 minus of x 1, correct. F b equal to f a 0 times x 1 minus of x 2, correct; f c equal to f a 0 times x 2 minus of x 3, okay, and f d equal to f a 0 times x 3, yes or no, what are we saying? What we are saying is that it is a multiple reaction; there are only three independent reactions. It is obvious; I have not proved it to you three is independent reactions. If x 1 x 2 x 3 are the extents of these reactions, this is the stoicheometry, and it means what?

It means that since they are all in equilibrium, you know that c b by c a is k 1, c c by c b is k 2, c d by c c is k 3, yes or no; this is the definition of equilibrium, we know this. Now since we know these three, now we can using this relationship since k 1 k 2 k 3 are given; since, k 1 k 2 are given, we should be able to find out x 1 x 2 x 3. There are three equations three unknowns; we should be able to find out.

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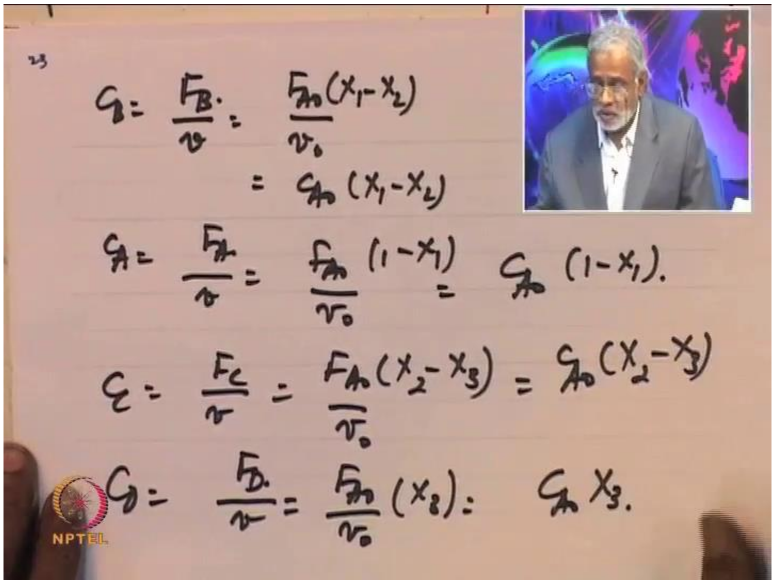

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$$C_B = \frac{F_B}{v} = \frac{F_{A0}(x_1 - x_2)}{v_0} = C_{A0}(x_1 - x_2)$$

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1 - x_1)}{v_0} = C_{A0}(1 - x_1).$$

$$C_C = \frac{F_C}{v} = \frac{F_{A0}(x_2 - x_3)}{v_0} = C_{A0}(x_2 - x_3)$$

$$C_D = \frac{F_D}{v} = \frac{F_{A0}}{v_0}(x_3) = C_{A0}x_3.$$

Let us do that, so that we know what the numbers are. So, help me now; what is c b? C b by definition c b equal to f b divided by v; what is f b which is f a 0 times x 1 minus of x 2. What is v? V equal to v 0 which is c a 0 times x 1 minus of x 2. Similarly, c a which is f a divided by v which is f a 0 times 1 minus of x 1 divided by v 0 which is c a 0 times 1 minus of x 1. Similarly, cc which is f c divided by v which is f a 0 times; what is f c, notice here what is f c? F c is x 2 minus of x 3, okay. So, we can put it here which is x 2 minus of x 3 divided by v 0; that is equal to c a 0 times x 2 minus of x 3, and then c d is what? F d divided by v which is f a 0 divided by v 0 into x 3 which is c a 0 times x 3, is that clear. Now what it means is that now we know from our problem statement, they are all in equilibrium; therefore, c b by c a is k 1. Therefore, from each of these equations we can determine and solve.

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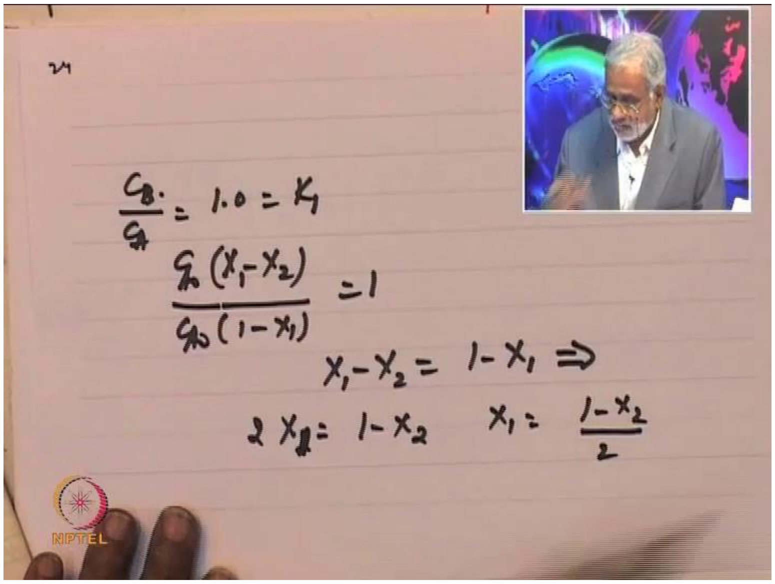

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$$\frac{C_B}{C_A} = 1.0 = K_1$$

$$\frac{C_{A0}(X_1 - X_2)}{C_{A0}(1 - X_1)} = 1$$

$$X_1 - X_2 = 1 - X_1 \Rightarrow$$

$$2X_1 = 1 - X_2 \qquad X_1 = \frac{1 - X_2}{2}$$

Let us do that quickly; so what are we having? C b by c a is k 1; k 1 is 1, okay, equal to k 1. C b is what? C a 0 times x 1 minus of x 2; c a is c a 0 times 1 minus of x 1 equal to 1 or x 1 minus of x 2 equal to 1 minus of x 1 that is equal to what do you get? X 2 equal to or x 1 we will say x 1 equal to 2 x 1 equal to correct; 2 x 1 is equal to 1 minus of x 2 or x 1 equal to 1 minus of x 2 by 2, okay.

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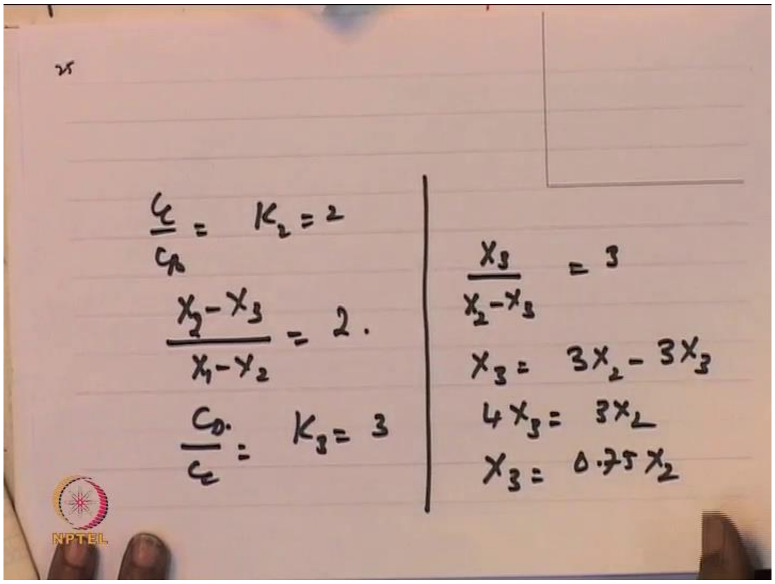

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$$\frac{C_C}{C_B} = K_2 = 2$$

$$\frac{X_2 - X_3}{X_1 - X_2} = 2.$$

$$\frac{C_D}{C_C} = K_3 = 3$$

$$\frac{X_3}{X_2 - X_3} = 3$$

$$X_3 = 3X_2 - 3X_3$$

$$4X_3 = 3X_2$$

$$X_3 = 0.75X_2$$

Now we can substitute this in the next equation, then second. Now we have c c by c b equal to k 2 equal to 2; c c is x 2 minus of x 3 divided by x 1 minus of x 2 that is equal to 2. Similarly, c d c d is what? C d by c c equal to k 3 equal to 3; so that gives as c d is what? X 3 divided by c c is x 2 minus of x 3 equal to 3. So, let us three have x 3 equal to 3 x 2 minus of 3 x 3; therefore, 4 x 3 equal to 3 x 2. So, x 3 equal to 0.75 x 2, okay. Now we can we can use this result, okay.

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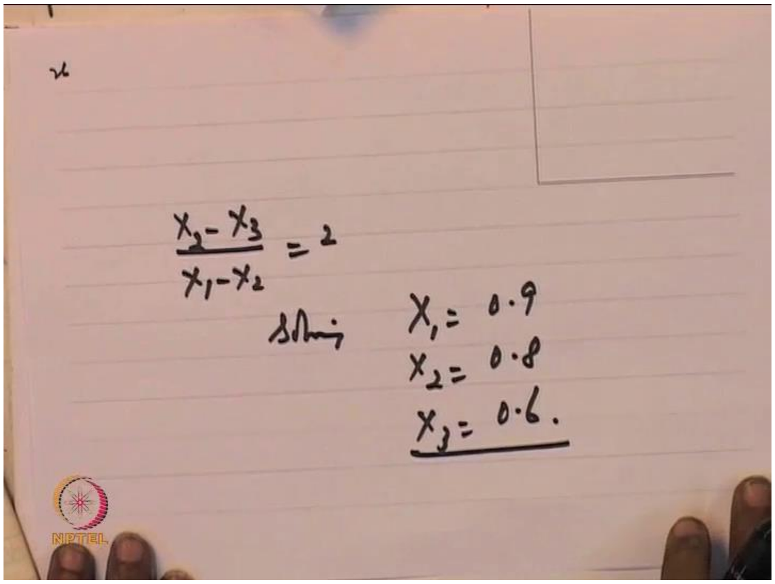

$$\frac{x_2 - x_3}{x_1 - x_2} = 2$$

Solving $x_1 = 0.9$

$x_2 = 0.8$

$x_3 = 0.6.$

So, we have x 2 minus of x 3 divided by x 1 minus of x 2 equal to 2 and then we have in the sense I will not do this now because it is fairly elementary. So, solving we get x 1 equal to 0.9; x 2 equal to 0.8; x 3 equal to 0.6. This is something that comes out of our, okay; so we will stop here and there is little bit more to be done. We will have to take it up when we meet next time. Thank you very much.