Advanced Chemical Reaction Engineering
Department of Chemical Engineering
Indian Institute of Technology, Bombay

Lecture - 7
Illustrative Examples 1 Recycle Reactor with condenser
2 CSTR with Recycle

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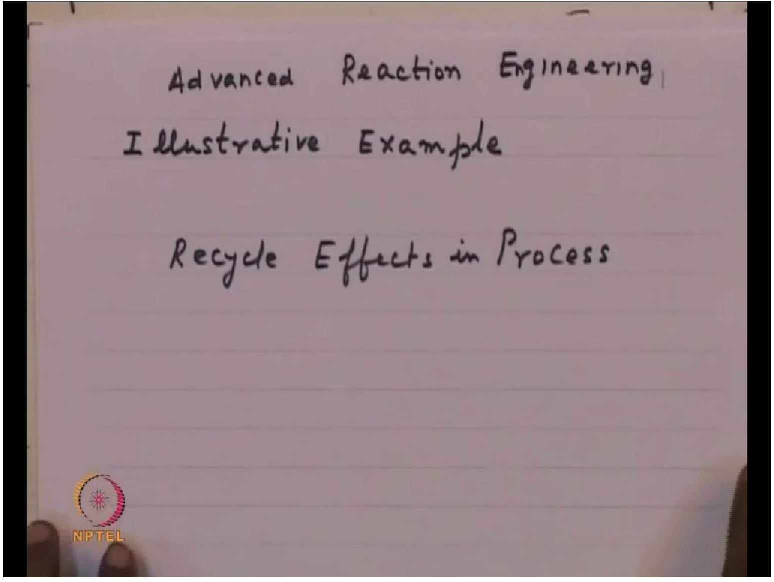

Advanced Reaction Engineering

Illustrative Example

Recycle Effects in Process

We look at recycle effects in process in this lecture. We will take some examples to illustrate and go through the numbers to illustrate how we can take care of recycle and what kind of effects they will produce.

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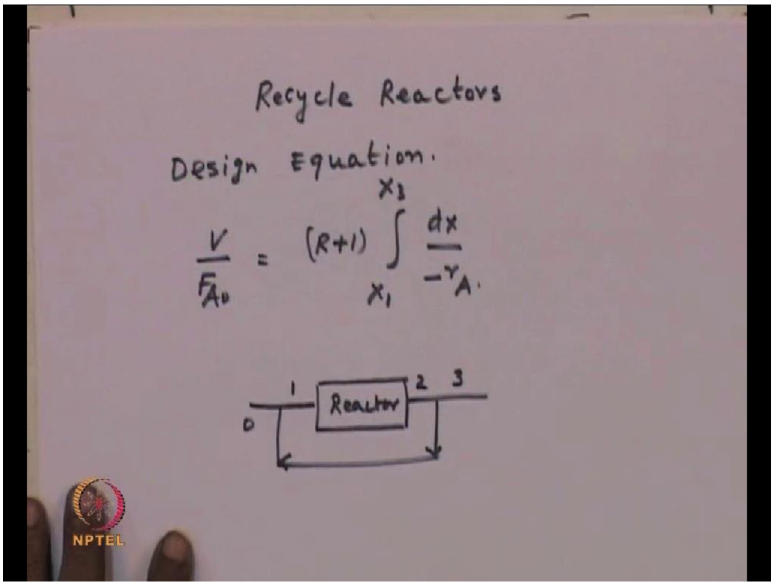

Recycle Reactors

Design Equation.

$$\frac{V}{F_{A0}} = (R+1)\int_{x_1}^{x_3} \frac{dx}{-r_A}.$$

We have talked about design equation for recycle reactor where, we said that the reactor volume v is given by this integral, where dx by minus of ra; ra is the rate function.

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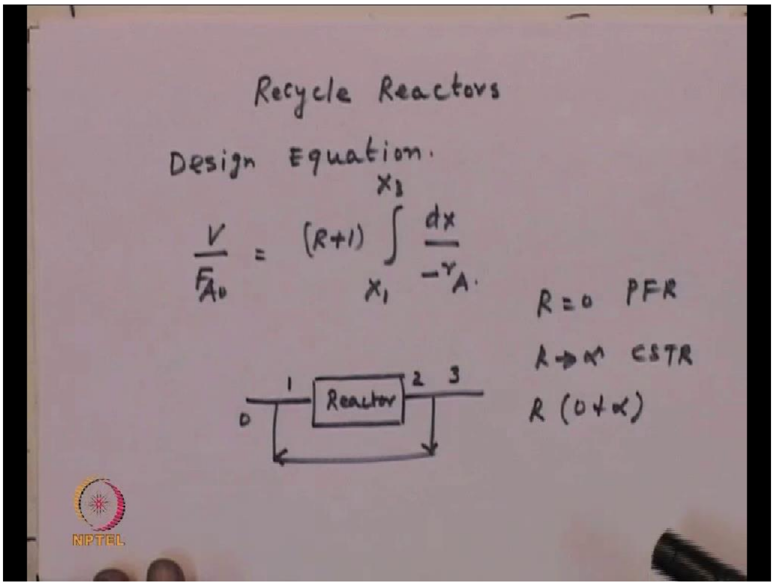

Recycle Reactors

Design Equation.

$$\frac{V}{F_{A0}} = (R+1)\int_{X_1}^{X_3} \frac{dx}{-r_A}.$$

$R = 0$ PFR

$R \to \infty$ CSTR

$R\ (0 + \infty)$

While doing this, we also said that when R, value of R is 0 and we get PFR or plug flow recycle reactor, when R is tending to infinity, very large, we get a CSTR and therefore, R in between 0 and infinity; you are able to approximate various types of devices, which lie between a PFR and the CSTR. If you look up on CSTR as a very well mixed vessel and PFR as where, there is no mixing; recycle is one way of approximating any type of reactor, which lies between a PFR and a CSTR; no mixing to very large amount of mixing. So, that is the great advantage of CSTR that you can get various degrees of mixing and therefore, appropriately, take care of the requirements of a process.

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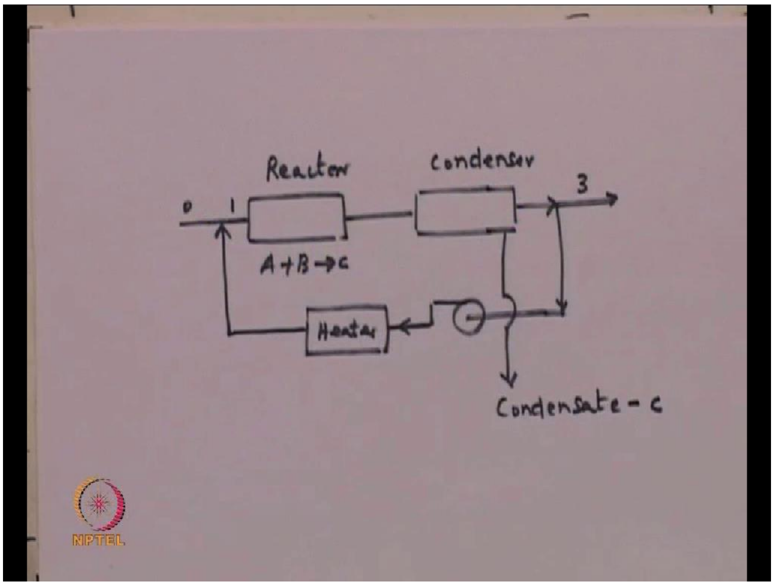

Now, what we would like to do today is to look at some examples where, recycles become important. Say for example, if you have a reaction A plus B going to C, and C is a condensable gas; you would condense this gas, and then collect this C, and then recycle and reacted material back into the process. We may not; this streams C, may be there, may not be there. Now, the fact that this happens that the certain amount of condensate comes out and the recycle is affected by the condenser; we will have to take into account how the reactor design takes into account, the effect of the condensate which, you will take an example to illustrate.

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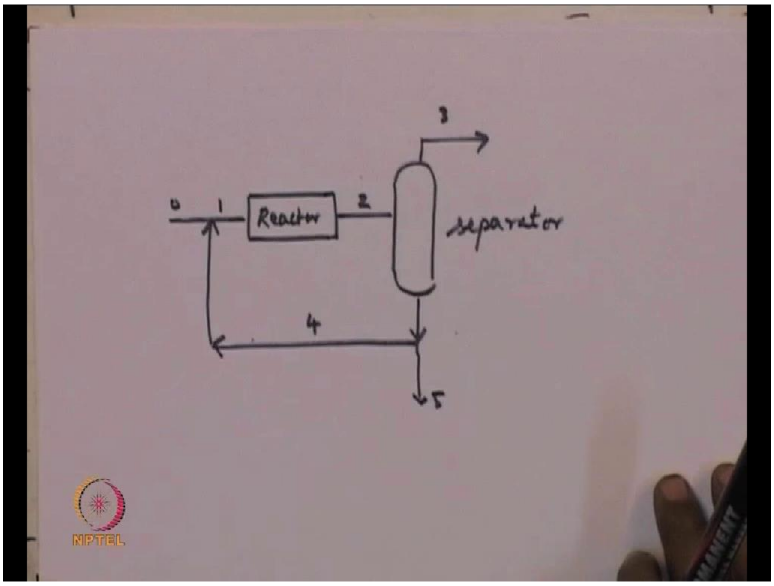

Now, there could be another situation that we will encounter. In fact, this is the most common kind of situation where, you have a reactor where, let us say reaction A going to B plus whatever; let us say A plus B going to C; whatever might be the situation. Now, we have a separator where, we remove the product, and then we recycle the unreacted. This reactor need not be a recycle; means, it can be a CSTR.

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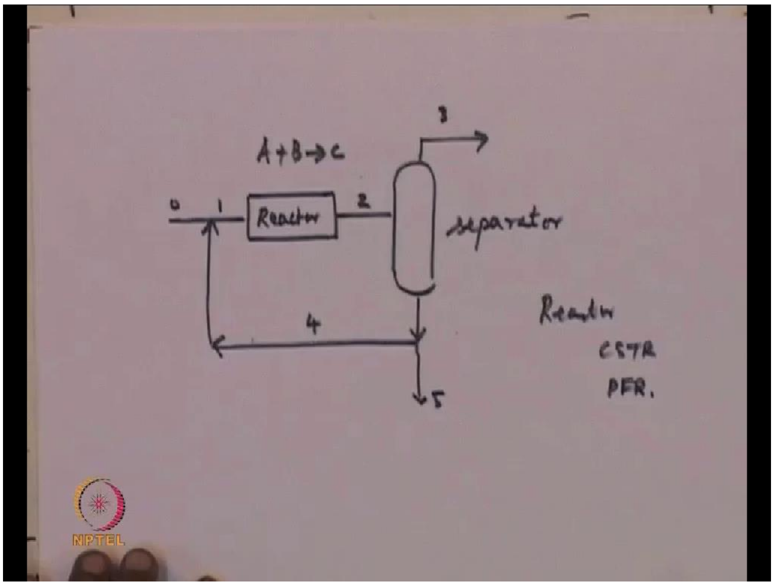

This reactor can be, for example, a CSTR or it might be a PFR or whatever, might be the situation of your interest. So, what we would like to do is to take some examples of these two situations, and then go through the numbers to understand, what are the new features that they bring into the process.

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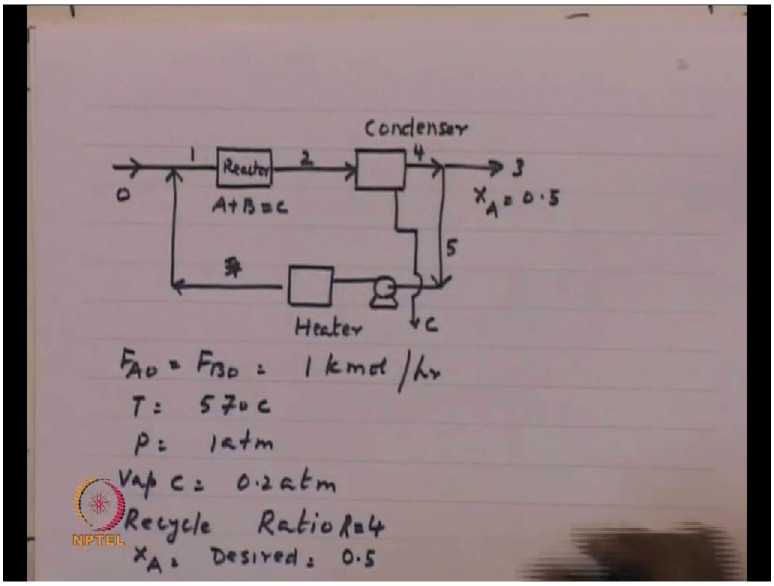

$F_{A0} = F_{B0} = 1$ kmol/hr
T: 570 c
P: 1atm
Vap C: 0.2atm
Recycle Ratio R=4
x_A: Desired: 0.5

First example I have taken here, is A plus B going to C. Reaction takes place at 570 c, at pressure of 1 atmosphere, and the vapor pressure of C is about 0.2 atmosphere, showing that it has a finite vapor pressure at 45; this is at 45 c. On other words, you have to condense; means, you have to cool, before we can condense C. The example I have taken is the desired conversion is 0.5, and then we recycle part of it where, the recycle ratio is given as 4. There could be examples in which, the stream 3 might not be there, so that, we actually, recycle a substantial part. To be able to look at the numbers, we will have to go through elements of stoichiometry which, you all understand.

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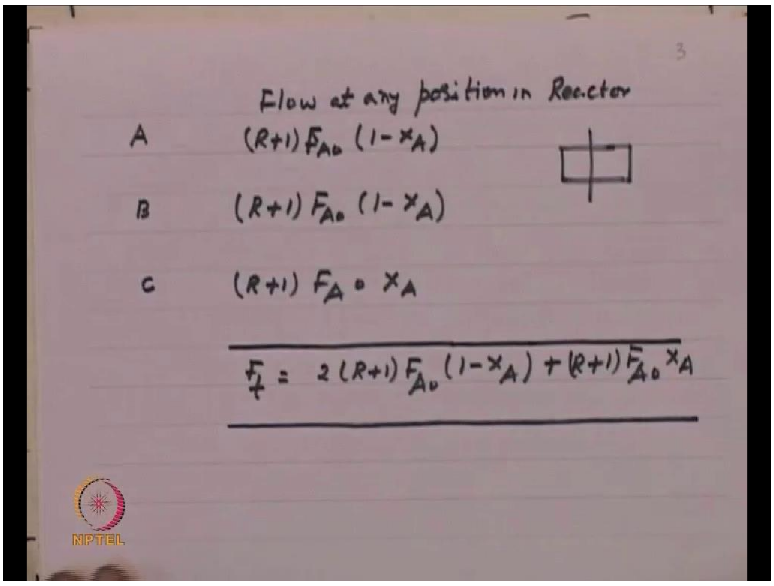

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Flow at any position in Reactor

A $(R+1)F_{A0}(1-x_A)$

B $(R+1)F_{A0}(1-x_A)$

C $(R+1)F_{A0}\,x_A$

$$F_t = 2(R+1)F_{A0}(1-x_A) + (R+1)F_{A0}x_A$$

At any position inside the reactor, which means, we have this reaction equipment. This is the reaction equipment, and then at any position in the reaction equipment, we say that if the recycle ratio is R, R plus one times F a 0, multiplied by 1 minus of X a would be the molar flow at this point. Since, A and B is taken as equi molar in this particular problem, A and B are taken as equi molar and therefore, B is also R plus 1 F a 0, 1 minus X a and see, the amount of product formed if X a is the extent of reaction, R plus 1 F a 0 X a is the amount of product that is formed. So, if we add up all these, you will get the total molar flow at any point in the equipment is as what I have written here; two times R plus 1. You can add these two here; two times R plus 1 F a 0, and then R plus 1 F a 0 F x. So, this is the total molar flow at any point in the equipment.

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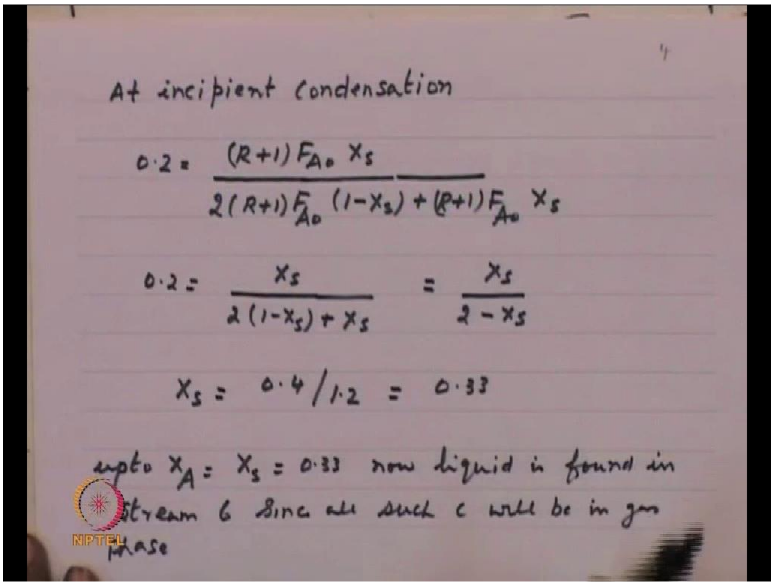

At incipient condensation

$$0.2 = \frac{(R+1)F_{A0}\, X_s}{2(R+1)F_{A0}(1-X_s) + (R+1)F_{A0}\, X_s}$$

$$0.2 = \frac{X_s}{2(1-X_s)+X_s} = \frac{X_s}{2-X_s}$$

$$X_s = 0.4/1.2 = 0.33$$

upto $X_A = X_s = 0.33$ now liquid is found in stream 6 since all such C will be in gas phase

Now, what we have said is that component C is a condensable gas. Therefore, it would condense and we can find out when the condensation occurs by putting this condition that at the point of incipient condensation; that means, at the point of incipient condensation, we have the mole fraction of component C, because total pressure is 1 atmosphere at p, is 1 atmosphere and vapor pressure of C, P star of C is 0.2 atmospheres.

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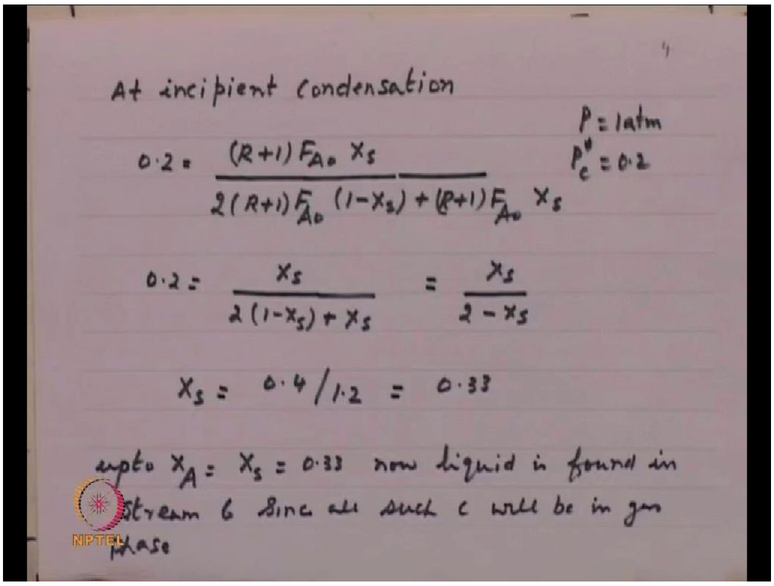

At incipient condensation

$P = 1 atm$

$P_c^* = 0.2$

$$0.2 = \frac{(R+1)F_{A0}\, X_s}{2(R+1)F_{A0}(1-X_s) + (R+1)F_{A0}\, X_s}$$

$$0.2 = \frac{X_s}{2(1-X_s)+X_s} = \frac{X_s}{2-X_s}$$

$$X_s = 0.4/1.2 = 0.33$$

upto $X_A = X_s = 0.33$ now liquid is found in stream 6 since all such C will be in gas phase

Therefore, when it becomes mole fraction equal to 0.2, it would condense. Therefore, we have, based on this stoichiometry, that this relationship should hold where, X s is the conversion at which, the condensation begins to take place. So, if you solve this and find that X s equal to 0.33 at X s equal to 0.33, condensation would begin. On other words, beyond the value of X s equal to 0.33, you will find that all the C condenses and therefore, in the gas phase, the value of C will not be more than X s. That is the important point which, we must take into account in the design of the equipment.

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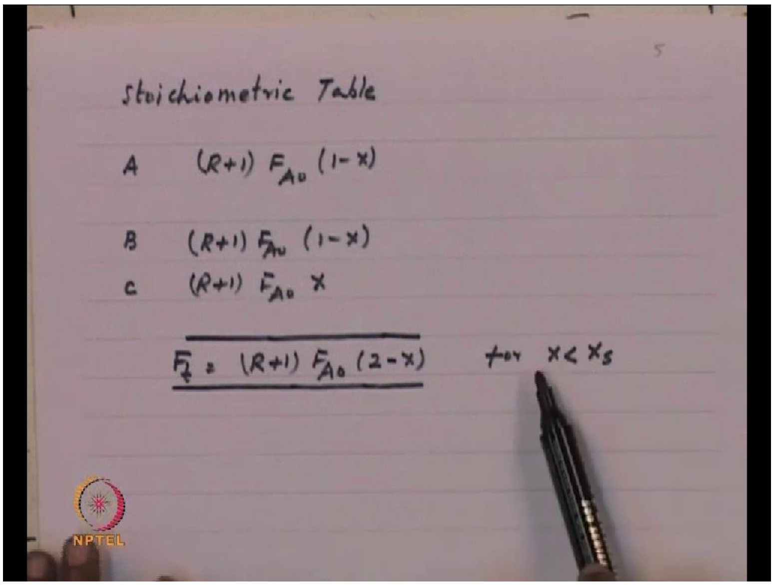

Stoichiometric Table

A $(R+1) F_{A0} (1-x)$

B $(R+1) F_{A0} (1-x)$

C $(R+1) F_{A0} x$

$F_T = (R+1) F_{A0} (2-x)$ for $x < x_s$

Let us see how it shapes up as we go along. So, what is the stoichiometric table for X less than X s? There is no condensation. Therefore, A is R plus 1 F a 0, 1 minus of X; B is R plus 1 F a 0, 1 minus X, because A and B are equi molar, and all the C that is formed, stays in the gas phase. Therefore, R plus 1, (( )) all of them are in the gas phase.

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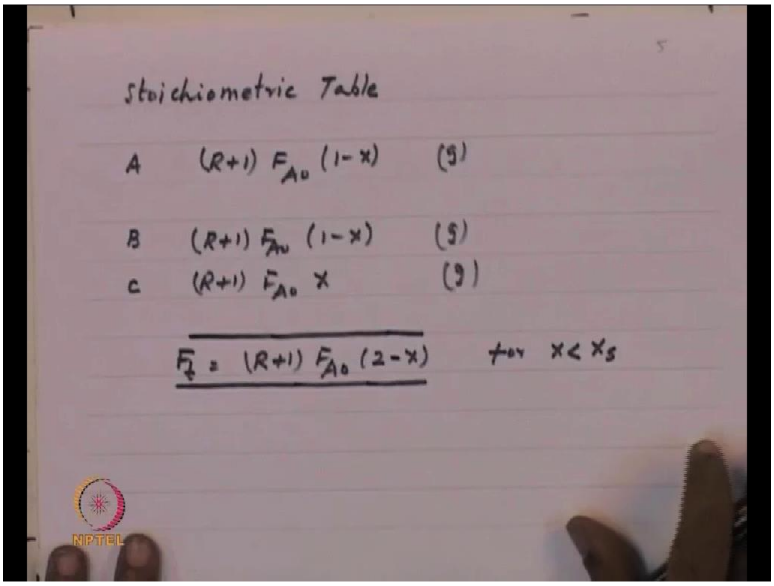

Stoichiometric Table

A $(R+1) F_{A0} (1-x)$ (g)

B $(R+1) F_{A0} (1-x)$ (g)

C $(R+1) F_{A0} x$ (g)

$F_T = (R+1) F_{A0} (2-x)$ for $x < x_s$

Therefore, the total molar flow becomes R plus 1 times F a 0 times 2 minus of X; this is for X less than X s. Now, when X becomes greater than X s, what happens?

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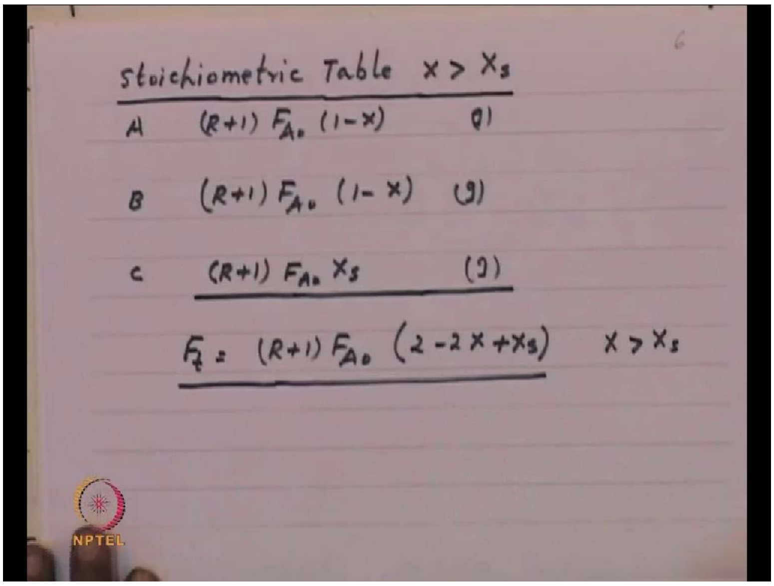

Stoichiometric Table $X > X_s$

A	$(R+1)F_{A0}(1-X)$	(1)
B	$(R+1)F_{A0}(1-X)$	(1)
C	$(R+1)F_{A0}X_s$	(1)

$$F_t = (R+1)F_{A0}(2-2X+X_s) \quad X > X_s$$

We have here, A and B are the same, and C; what happens is that C R plus 1 F a 0 X s and beyond that, C does not go into the gas phase. So, the highest amount of C in the gas phase is given by R plus 1 F a 0 X s. Therefore, the gas phase beyond X s equal to 0.5, condenses. Therefore, it ends, does not enter the gas phase. So, the total molar flow for the case of X greater than X s is given by this representation; F t equal to R plus 1 F a 0, 2 minus of 2 X plus X s.

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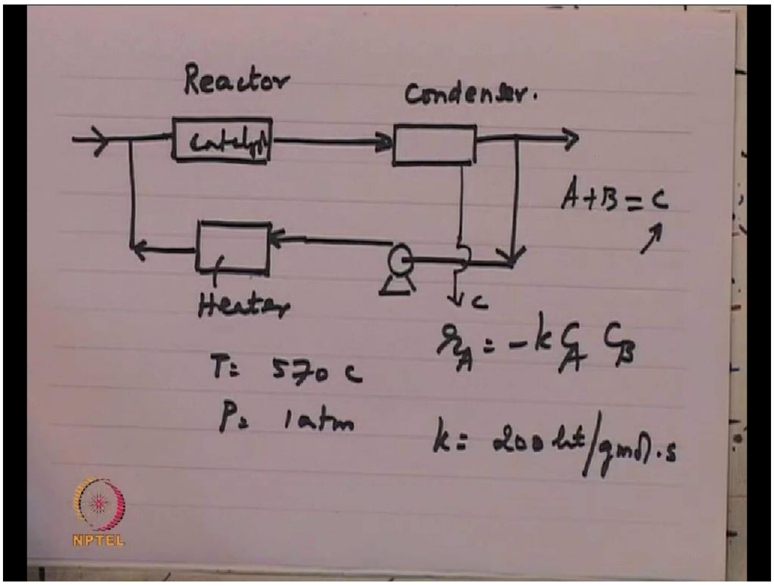

$T = 570\ C$

$P = 1\ atm$

$r_A = -k C_A C_B$

$k = 200\ lit/gmol \cdot s$

Now, what we want to do is to recognize that reaction A plus B going to C where, C is a condensable gas and even, the reaction rate constant of 200 liter per gram mole second. So, we have a catalytic reaction; a catalyst here, and then we are recycling it, and recycling after removal of the condensate; this is condensate C. Once again, recognize that the condensate stream 1, still it starts to condense; till it becomes saturated, it does not condense. Basically, that is a point that we have to take into account. Now, we have said all these.

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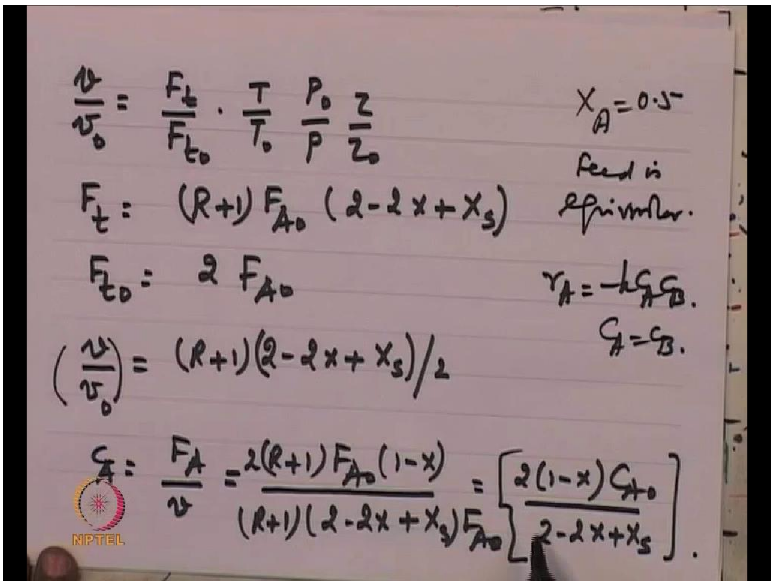

$$\frac{v}{v_0} = \frac{F_t}{F_{t0}} \cdot \frac{T}{T_0} \frac{P_0}{P} \frac{Z}{Z_0}$$

$X_A = 0.5$

Feed is equimolar.

$$F_t = (R+1) F_{A0} (2 - 2x + X_s)$$

$$F_{t0} = 2 F_{A0}$$

$r_A = -k C_A C_B.$

$C_A = C_B.$

$$\left(\frac{v}{v_0}\right) = (R+1)(2 - 2x + x_s)/2$$

$$C_A = \frac{F_A}{v} = \frac{2(R+1) F_{A0} (1-x)}{(R+1)(2 - 2x + X_s) F_{A0}} = \left[\frac{2(1-x) C_{A0}}{2 - 2x + x_s}\right].$$

So, we quickly, recognize that for the case of condenser for X a equal to 0.5 conversion, by gas law, we get v by v 0 is this; the total molar flow, all those details, we have done. Therefore, we can get the total, the volumetric flow is given by this. Therefore, the concentration that is given by simple expressions like this. On other words, if our rate expression is minus of kcacb, now, we can substitute for ca and cb. In this case, ca equal to cb, because the feed is equi molar. Therefore, we can substitute for ca and cb in this rate expression, and then integrate to find out what is the size of the equipment that is required. We have done this. I am doing this again just to bring to your attention an important feature.

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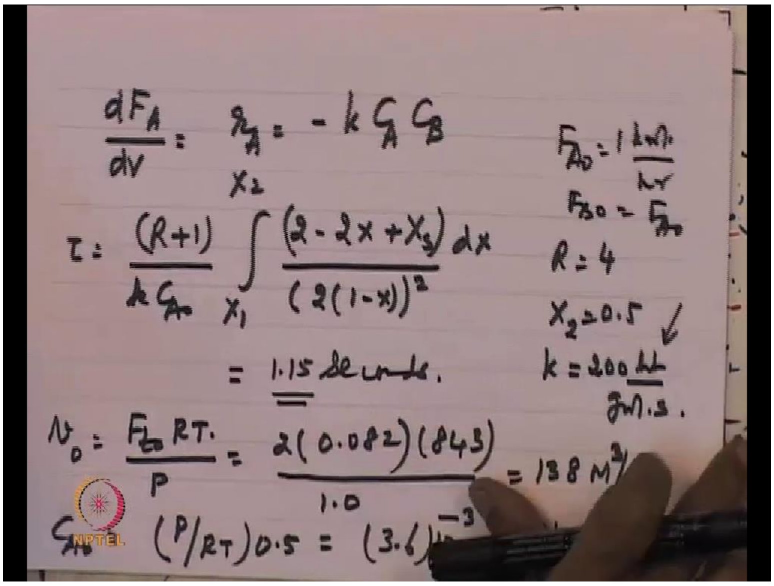

$$\frac{dF_A}{dV} = r_A = -k C_A C_B$$

$$\tau = \frac{(R+1)}{k C_{A0}} \int_{X_1}^{X_2} \frac{(2-2X+X_3)}{(2(1-X))^2}\,dX$$

$$= \underline{\underline{1.15}}\ \text{seconds.}$$

$$v_0 = \frac{F_{t0} RT}{P} = \frac{2(0.082)(843)}{1.0} = 138\ M^3/$$

$$C_{A0} = (P/RT)0.5 = (3.6)\,{}^{-3}$$

$F_{A0} = 1\ \frac{kmol}{hr}$

$F_{B0} = F_{A0}$

$R = 4$

$X_2 = 0.5$

$k = 200\ \frac{lit}{gmol.s}.$

That means, we can find the residence time; we can we find the mole of flow rate at the inlet is 138 cubic meters; concentration of the inlet is 3.6 of 10 minus 3. Now, if the reaction rate is 200 liters per gram mole second, then we can find out and based on this calculation, that the residence time is 1.15 seconds; that means, if the reaction rate is as high as 200 liters per gram mole second, then the residence times becomes 1.15 seconds. On other words, for this flow rate, if F a 0 equal to 1 kilo mole per hour, and then and F b 0 equal to F a 0; if this is the situation, then we can find out that there is the residence time that is required to process this is 1.15 seconds.

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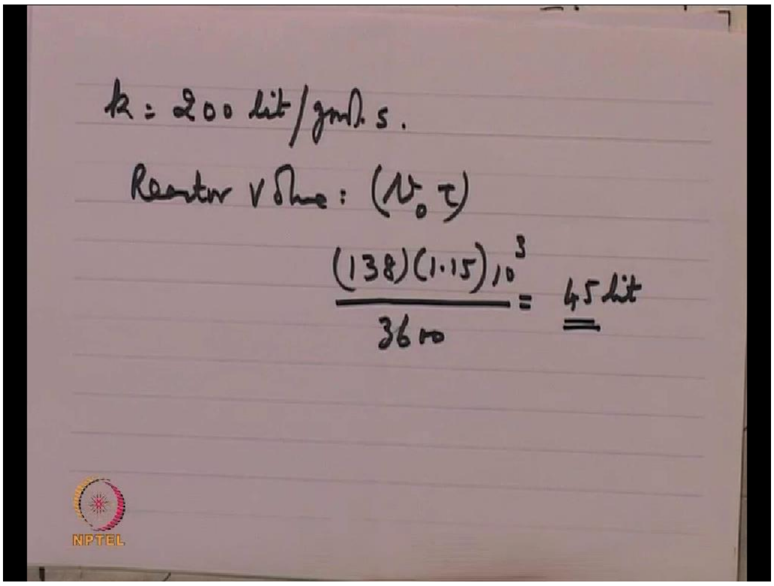

$k = 200\ \text{lit/gmol s}.$

Reactor volume: $(v_0 \tau)$

$$\frac{(138)(1.15)\,10^3}{3600} = \underline{\underline{45\ \text{lit}}}$$

Therefore, the size of the equipment that is required to process 1 kilo mole per is 45 liters.

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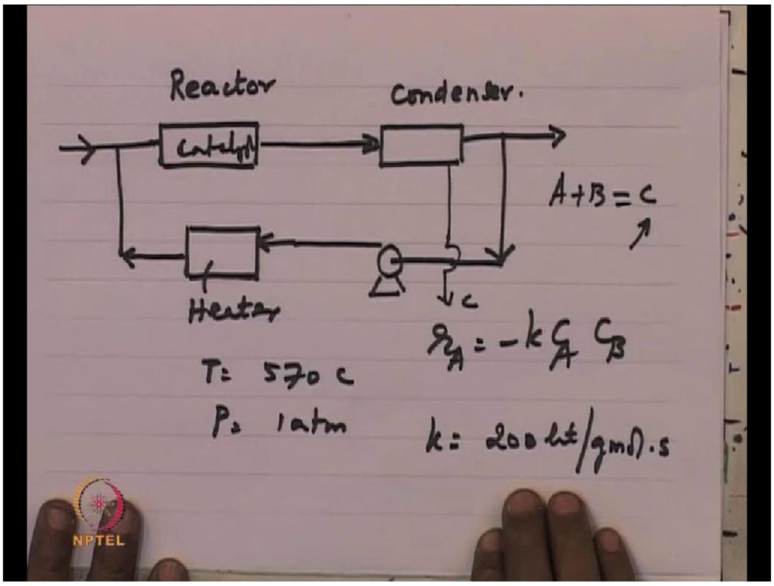

What are we saying; what we are trying to say here, is the following; we have a reaction A plus B going to C, and then this C is a condensable gas, and then as a result of which, you find that this stream, the recycle stream; only after, it is saturated, that condensation begins, and that effect of that condenser; we have taken into account through the procedure that we have set out. When these reaction rate constants are as high as 200 liters per gram mole second, we have just now, shown that the size of the reactor required is about 45 (( )). Now, point that perhaps, is relevant to recognize is the following.

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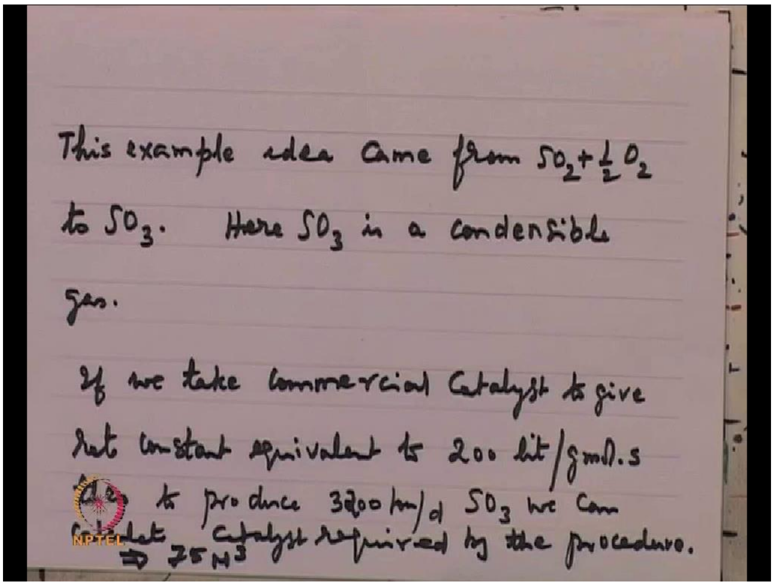

This example idea came from $SO_2 + \frac{1}{2} O_2$ to SO_3. Here SO_3 in a condensible gas.

If we take commercial catalyst to give rate constant equivalent to 200 lit/gmol.s Also to produce 3200 ton/d SO_3 we can calculate catalyst required by the procedure.
⇒ 75 m^3

That is I mean, this whole example has been taken, being inspired by what happen in this sulfur dioxide plant. Sulfur trioxide is a condensable gas; it has a vapor pressure, I mean at 45 degrees is the significant degree of vapor pressure and so on. Now, if you are looking at a commercial catalyst and just making an estimate, whose rate of constant, let us say is 200 liter per gram mole second, then to produce something like 3200 tons per day of sulfur trioxide; we can easily calculate based on the numbers we have taken. It requires about 75 cubic meters of catalyst. On other words, what we are trying to say is that a plant producing about 3200 tons per day of sulfur trioxide, will actually, use up about 75 cubic meters of catalyst. This is the kind of numbers that we have, I mean, that we estimate. Of course, what happens in reality, and so many other things may take place, but if the rate constant is 200 liters per gram mole second to produce 3200 tons per day, we will need about 75 cubic liters of catalyst. That is the point we are trying to get across.

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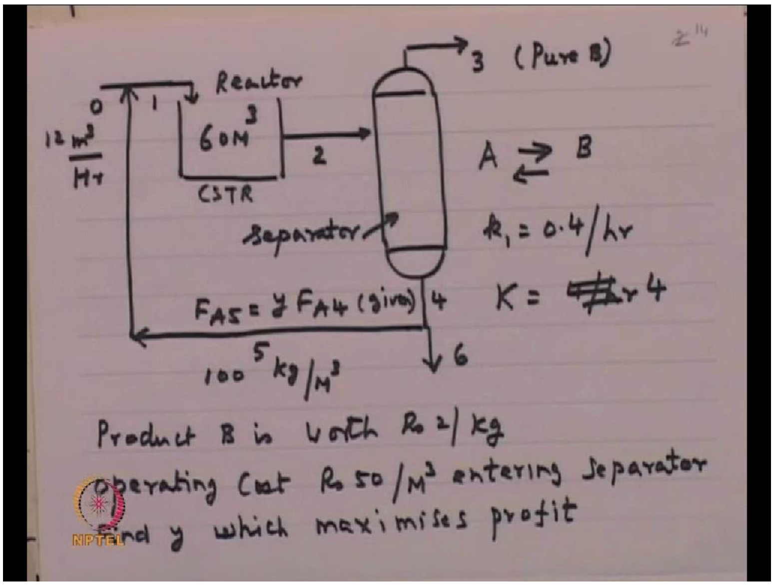

Product B is worth Rs 2/kg

Operating Cost Rs 50/M^3 entering Separator

Find y which maximises profit

The second example which, you would like to look at is also, a very common, as you see in the process industry. The example I have taken here is a stirred tank. This is the CSTR in this stirred tank, and after the reaction, it goes to a separator where, the product, the reaction A goes to B, is reversible; rate constants are given; equilibrium constant is given, and in this separator, product B is completely recovered, and the un reactor is recycled. But since, product B is recovered, the concentrations here, may not be satisfactory. Therefore, you make up the concentrations in this stream and make it up to 100 kg per cubic meter, as for specified in this exercise and this recycle, so that, the concentration at position 1 is also equal to what we have in the fresh feed stream.

Now, the point we noticed here, in that as we try and put the unreacted material back into the process, there is a cost associated with separation, and therefore, this is the cost of separation that goes back into the process. Therefore, you will find, in general, the effect of this would be to give you a certain optimum at which, you must operate. Now, this optimum might be defined in various ways. In this particular exercise, we have taken optimum with respect to cost of running the process. There would be very other ways in which, you can define the objective function to do your optimization. In this particular case, just to illustrate what we might be able to do is to take the example of cost.

So, accordingly, in this particular problem, what is specified is there is a process in which, 12 cubic meters per hour of component A is entering the process, and it is mixing with a recycle stream, which is suitably made up, so that, the concentrations are the same, and then after mixing, it enters the equipment. The reactor of volume 60 cubic meters is given as a stirred tank and the reactor, after reaction, it is entering a separator where, product B is completely recovered, and unreacted A is recycled after appropriate make up of the concentration streams. There is a stream 6, which is discarded. There is certain amount of stream 6, is discarded and what is said in this problem is a fraction y of stream 4 is recycled; not all of it is recycled; a fraction y is recycled. The idea is to find out what is the fraction y, which would be optimum from the point of view of cost of running this process. This is the exercise that we want to do. One of the part of the reasons why this example has been taken is that it illustrates how we understand the interaction between the reaction equipment and the separation equipment, because every process involving a reaction; you will find that you would separate a product and the cost of separation and the cost of reaction, and they have to be properly balanced, so that, your process runs satisfactorily.

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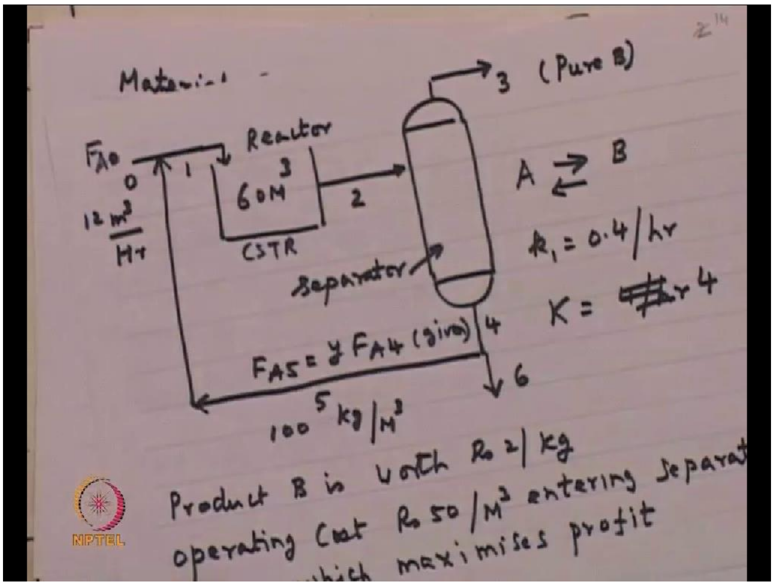

Product B is worth Rs 2/kg

operating Cost Rs 50/M^3 entering Separat

which maximises profit

Let us try and understand this problem in some. So, what we have said; to be able to solve this problem what we have done is we have done a material balance at position 1. What is happening at position 1? F a 0, if I call this stream K; F a 0 is entering; there is no B in the product. So, F a 0 is coming in and it is mixing with F a 5.

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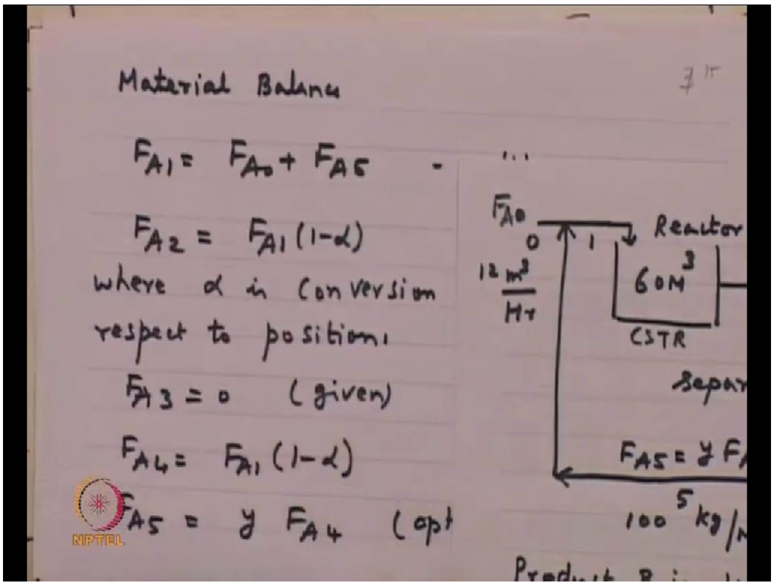

Material Balance

$F_{A1} = F_{A0} + F_{A5}$ ...

$F_{A2} = F_{A1}(1-\alpha)$

where α is conversion respect to position 1

$F_{A3} = 0$ (given)

$F_{A4} = F_{A1}(1-\alpha)$

$F_{A5} = y\,F_{A4}$ (opt

That is what is written here; F a 1 is F a 0 plus F a 5; statement of material balance. Now, since we are dealing with recycle, in this, we have defined conversions that take place in this equipment with respect to position 1. We find it convenient.

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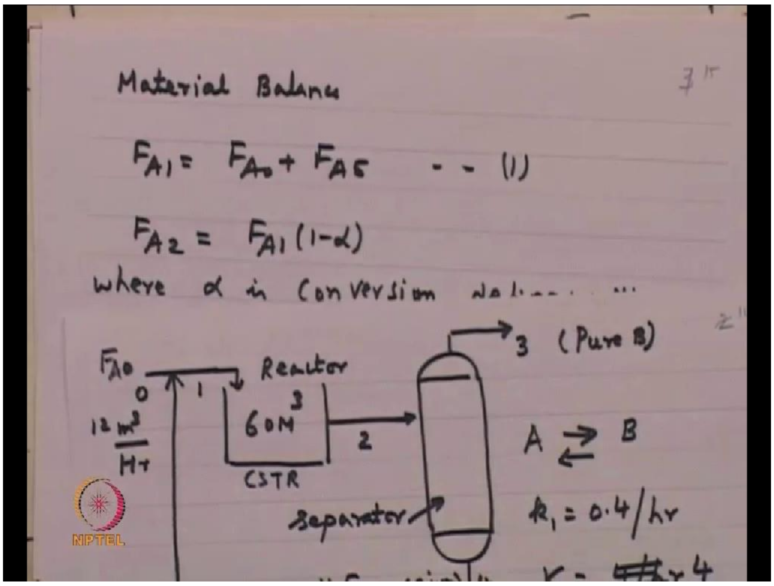

Material Balance

$F_{A1} = F_{A0} + F_{A5}$ -- (1)

$F_{A2} = F_{A1}(1-\alpha)$

where α is conversion w.r.t. ...

When you define conversion with respect to position 1, F a 2, as you can see here, becomes F a 1 times 1 minus of alpha; that means, a fraction alpha based on F a 1, has been consumed. That is what is stated here. So, fraction alpha of F a 1 is consumed.

Therefore, what emerges from the reaction equipment is the unreacted A, which is F a 1 times 1 minus of alpha. Therefore, the amount of reacted material is F a 1 times alpha; that it be the product B in this.

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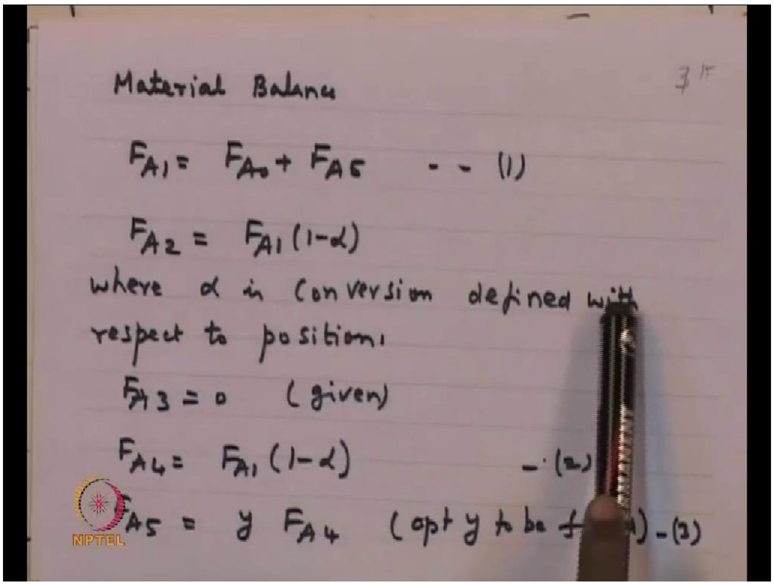

Material Balance

$F_{A1} = F_{A0} + F_{A5}$ -- (1)

$F_{A2} = F_{A1}(1-\alpha)$

where α is conversion defined with respect to position 1

$F_{A3} = 0$ (given)

$F_{A4} = F_{A1}(1-\alpha)$ -- (2)

$F_{A5} = y\, F_{A4}$ (opt y to be f) - (3)

We have defined conversion alpha, with respect to position 1; this is with respect to position 1; that means, with respect to F a 1. Now, what is also given is that F a 3, there is no product; there is no pure B.

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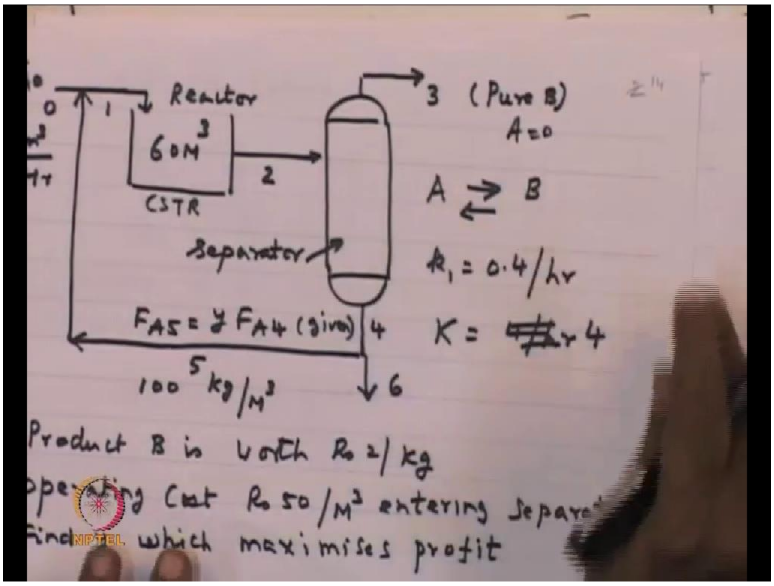

Product B is worth Rs 2/kg

Operating Cost Rs 50/M^3 entering Separa

Find which maximises profit

Therefore, A is 0 here; it is given. What is F a 4 where, F a 4 would be whatever is presenting F a 2, would come at F a 4.

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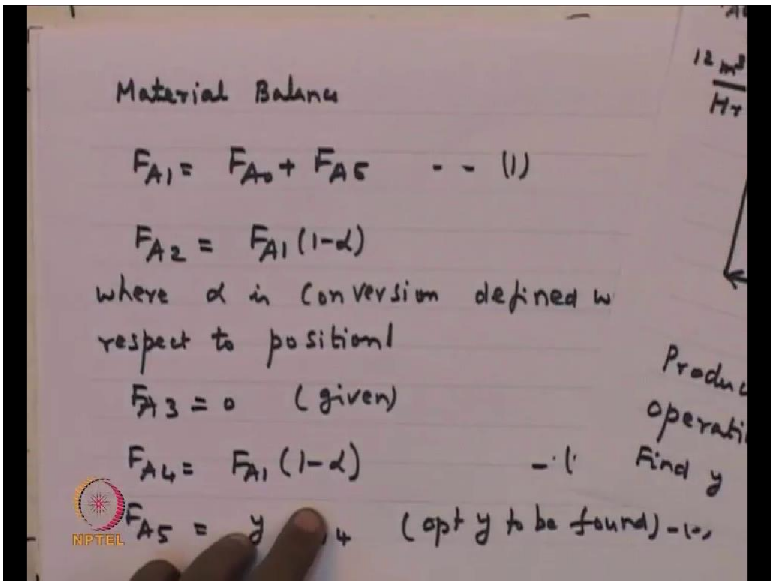

Material Balance

$F_{A1} = F_{A0} + F_{A5}$ -- (1)

$F_{A2} = F_{A1}(1-\alpha)$

where α is conversion defined w respect to position 1

$F_{A3} = 0$ (given)

$F_{A4} = F_{A1}(1-\alpha)$ -- (

$F_{A5} = y\ \ 4$ (opt y to be found) -- (

So, it is written as F a 1 times 1 minus of alpha. What is a F a 5? F a 5, by definition, fraction y of F a 4 is recycled.

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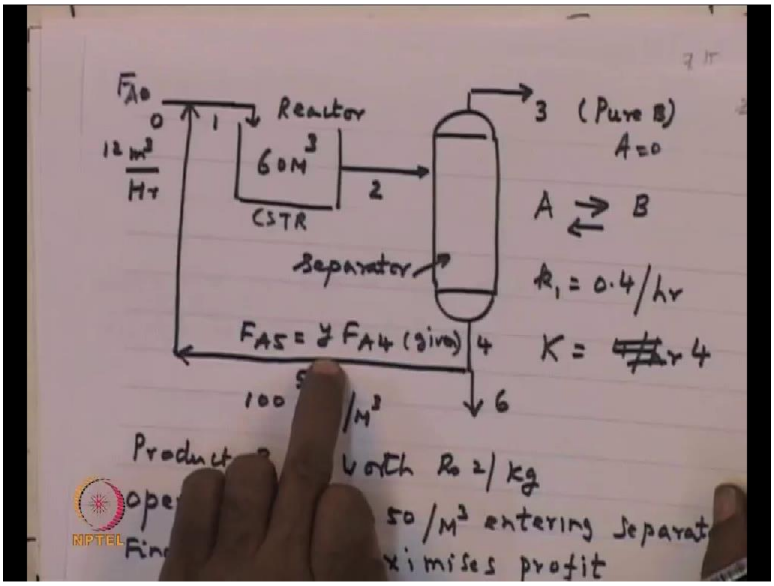

$A \rightleftarrows B$

$k_1 = 0.4/hr$

$K = 4$

Product B worth Rs 2/kg

Ope 50/M³ entering Separat

Fin ximises profit

So, y times F a 4 is recycled and our object is to find out the fraction y that would optimize the operation of this process. So, what are we saying now?

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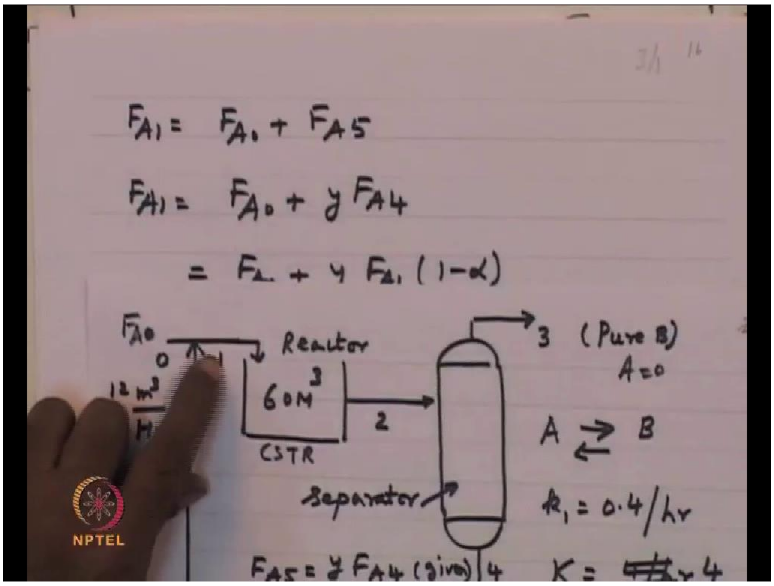

$$F_{A1} = F_{A0} + F_{A5}$$

$$F_{A1} = F_{A0} + y F_{A4}$$

$$= F_{A0} + y F_{A1}(1-\alpha)$$

What we are saying is that F a 1 is F a 0 plus F a 5.

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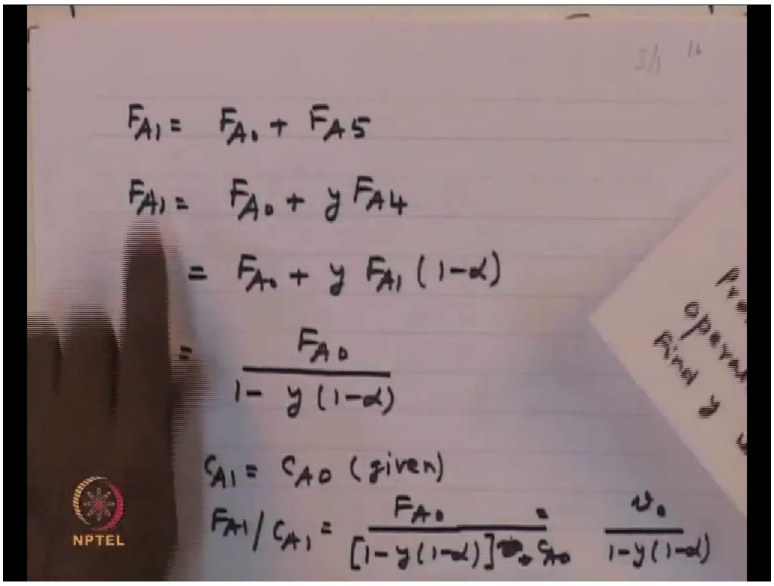

$$F_{A1} = F_{A0} + F_{A5}$$

$$F_{A1} = F_{A0} + y F_{A4}$$

$$= F_{A0} + y F_{A1}(1-\alpha)$$

$$= \frac{F_{A0}}{1 - y(1-\alpha)}$$

$$C_{A1} = C_{A0} \text{ (given)}$$

$$F_{A1}/C_{A1} = \frac{F_{A0}}{[1-y(1-\alpha)]\, C_{A0}} = \frac{v_0}{1-y(1-\alpha)}$$

It is what is mentioned here. Now F a 5 is fraction y of F a 4 is recycled. Therefore, y times F a 4 is F a 5 and we also said that F a 4, whatever is coming at 4 is what is present at position 2, which is F a 1 times 1 minus of alpha.

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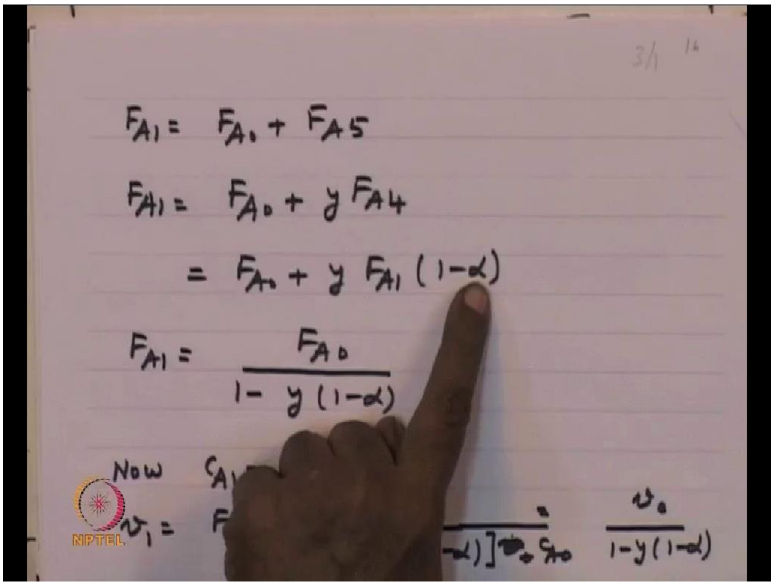

$$F_{A1} = F_{A0} + F_{A5}$$

$$F_{A1} = F_{A0} + y F_{A4}$$

$$= F_{A0} + y F_{A1} (1-\alpha)$$

$$F_{A1} = \frac{F_{A0}}{1 - y(1-\alpha)}$$

Now C_{A1}

$v_1 = F \quad -\alpha)] v_0 C_{A0} = \frac{v_0}{1-y(1-\alpha)}$

Therefore, we are put here, F a 1 times 1 minus of alpha. So, from this statement of material balance, what we find is that F a 1 is F a 0, divided by 1 minus of y times 1 minus of alpha.

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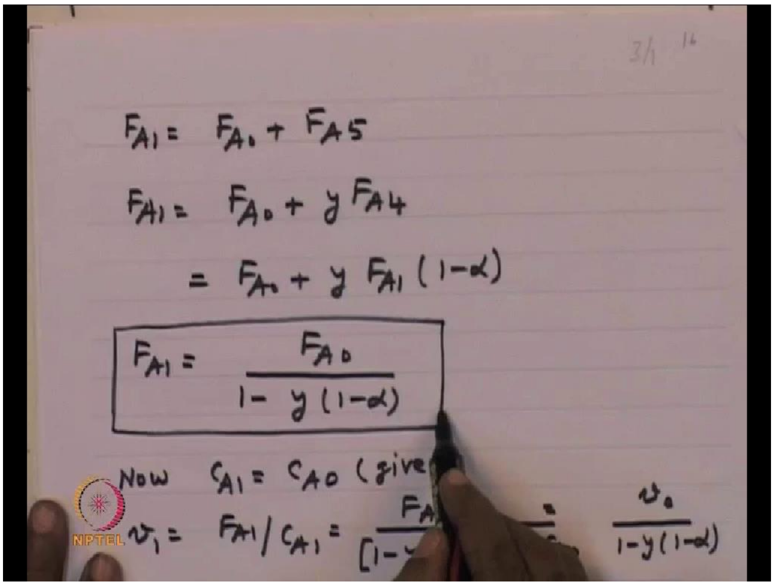

$$F_{A1} = F_{A0} + F_{A5}$$

$$F_{A1} = F_{A0} + y F_{A4}$$

$$= F_{A0} + y F_{A1} (1-\alpha)$$

$$\boxed{F_{A1} = \frac{F_{A0}}{1 - y(1-\alpha)}}$$

Now $C_{A1} = C_{A0}$ (give

$v_1 = F_{A1}/C_{A1} = \frac{F_{A}}{[1-} = \frac{v_0}{1-y(1-\alpha)}$

So, we are able to determine what is F a 1 in terms of the process variable. What are the process variable; y and alpha; see y and alpha are the variables of the process which, we have to find out what is the optimum value of y that would run the process well. Now, we have C a 1.

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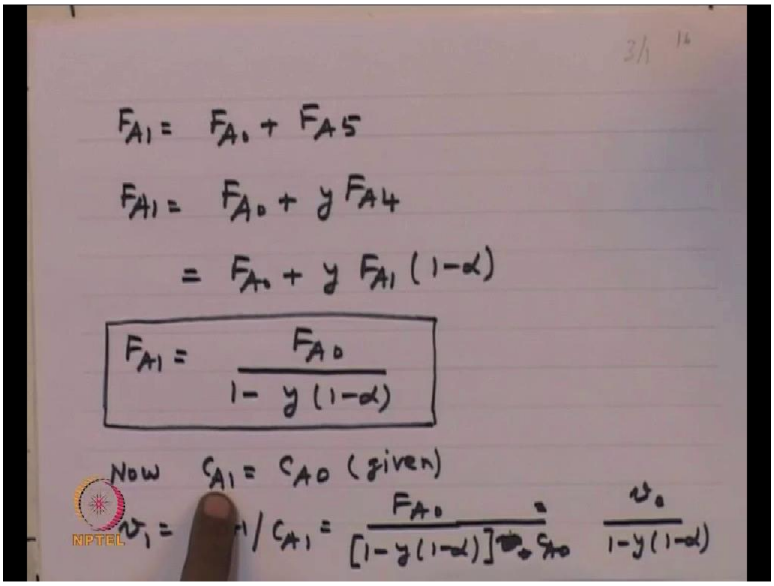

$F_{A1} = F_{A0} + F_{A5}$

$F_{A1} = F_{A0} + y F_{A4}$

$= F_{A0} + y F_{A1}(1-\alpha)$

$$\boxed{F_{A1} = \frac{F_{A0}}{1-y(1-\alpha)}}$$

Now $C_{A1} = C_{A0}$ (given)

$v_1 =$ [illegible]$_1/C_{A1} = \frac{F_{A0}}{[1-y(1-\alpha)]\,C_{A0}} = \frac{v_0}{1-y(1-\alpha)}$

What is C a 1? Feed is coming at C a 0 and this stream 5, as per the problem statement, it is made up, so that, the concentration here is same as concentration of the fresh feed stream.

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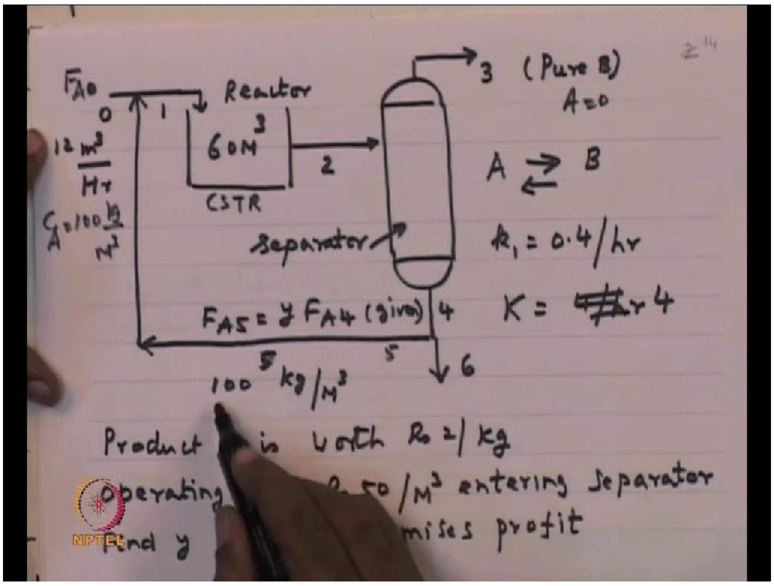

$A \rightleftarrows B$

$k_1 = 0.4/hr$

$K = 4$

Product is worth Rs 2/kg

Operating Rs 50/M^3 entering Separator

Find y mises profit

Fresh feed stream concentration is 100; it is given as 100 kg per cubic meter, and this stream is also made up, so that, it becomes 100 kg per cubic meter. This is stream 5. This also 100 kg per cubic meter; that is C a 5 is also 100 kg per cubic meter, so that, at position 1, our concentration is also 100 kg per cubic meter. That is what is being said here.

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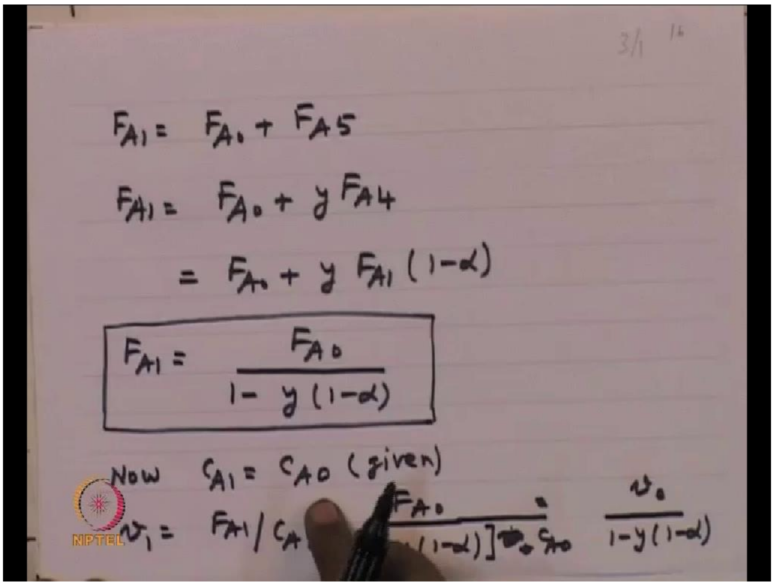

$F_{A1} = F_{A0} + F_{A5}$

$F_{A1} = F_{A0} + y F_{A4}$

$= F_{A0} + y F_{A1}(1-\alpha)$

$$\boxed{F_{A1} = \frac{F_{A0}}{1 - y(1-\alpha)}}$$

Now $C_{A1} = C_{A0}$ (given)

$v_1 = F_{A1}/C_{A}$ $\frac{F_{A0}}{(1-\alpha)]\, C_{A0}} = \frac{v_0}{1-y(1-\alpha)}$

Since, C a 1 is same as C a 0, what is v 1?

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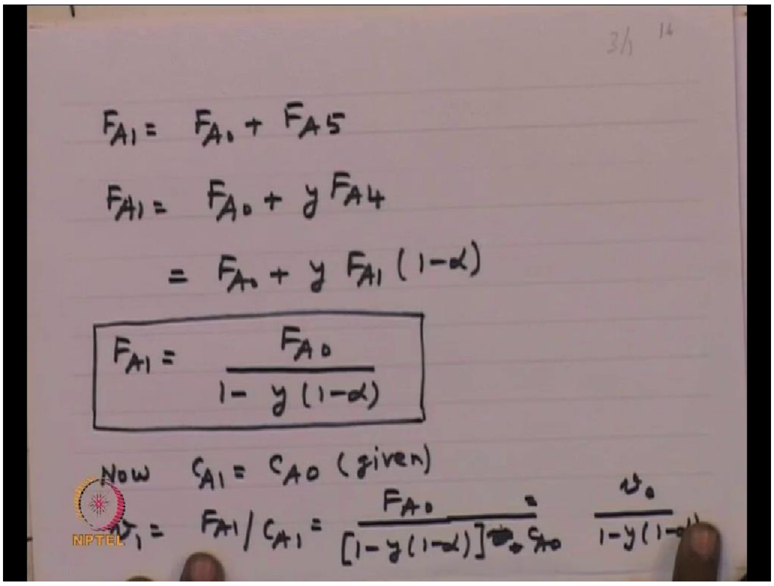

$F_{A1} = F_{A0} + F_{A5}$

$F_{A1} = F_{A0} + y F_{A4}$

$= F_{A0} + y F_{A1}(1-\alpha)$

$$\boxed{F_{A1} = \frac{F_{A0}}{1 - y(1-\alpha)}}$$

Now $C_{A1} = C_{A0}$ (given)

$v_1 = F_{A1}/C_{A1} = \frac{F_{A0}}{[1-y(1-\alpha)]\, C_{A0}} = \frac{v_0}{1-y(1-}$

Our first principle F a 1 by C a 1 is v 1. F a 1, we have just now found out is F a 0 times 1 minus of alpha. Therefore, we can replace C a 1 in terms of C a 0. Therefore, v 1 becomes v 0, divided by 1 minus of y times 1 minus of alpha. Interesting point here is that we are able to relate every variable of interest to us, in terms of parameters that we want to determine; y and alpha. We do not know y; we do not know alpha. So, our interest is to understand how y and alpha affect our process. In fact, every process that you run, you will find that these are the kinds of decisions that you have to make to get your process to work at the most optimum point.

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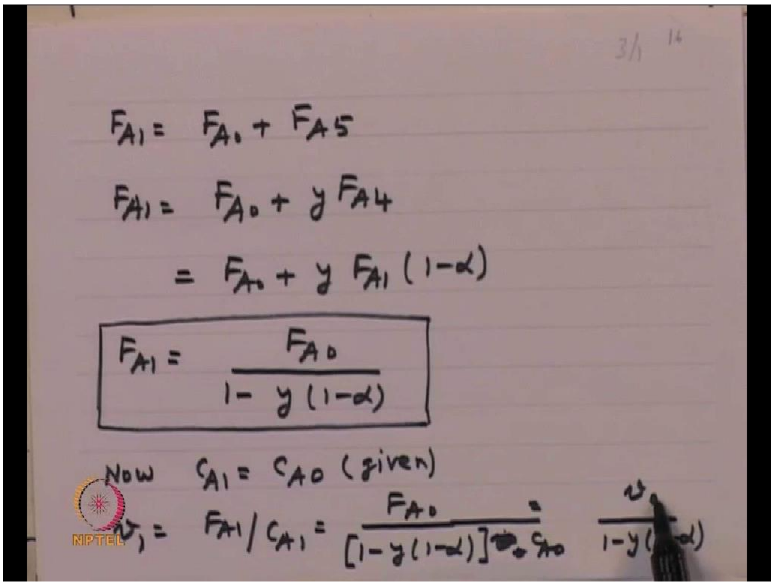

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$$F_{A1} = F_{A0} + F_{A5}$$

$$F_{A1} = F_{A0} + y F_{A4}$$

$$= F_{A0} + y F_{A1}(1-\alpha)$$

$$\boxed{F_{A1} = \frac{F_{A0}}{1-y(1-\alpha)}}$$

Now $C_{A1} = C_{A0}$ (given)

$$v_1 = F_{A1}/C_{A1} = \frac{F_{A0}}{[1-y(1-\alpha)]\,C_{A0}} = \frac{v_0}{1-y(1-\alpha)}$$

Once again, we (( )) molar flow rate as a volumetric flow at 1, is given now in terms of volumetric flow rate at 0, divided by 1 minus of y times 1 minus of alpha where, y and alpha are variables of our interest.

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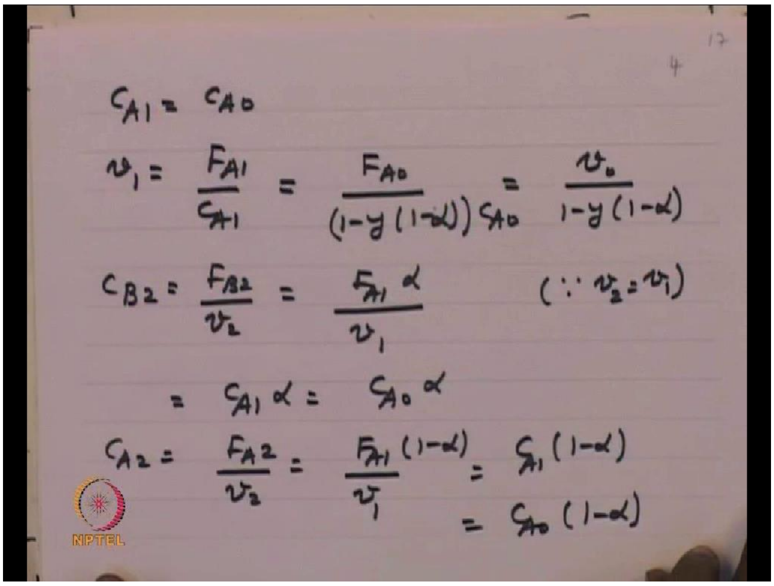

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$$C_{A1} = C_{A0}$$

$$v_1 = \frac{F_{A1}}{C_{A1}} = \frac{F_{A0}}{(1-y(1-\alpha))\,C_{A0}} = \frac{v_0}{1-y(1-\alpha)}$$

$$C_{B2} = \frac{F_{B2}}{v_2} = \frac{F_{A1}\,\alpha}{v_1} \qquad (\because v_2 = v_1)$$

$$= C_{A1}\,\alpha = C_{A0}\,\alpha$$

$$C_{A2} = \frac{F_{A2}}{v_2} = \frac{F_{A1}(1-\alpha)}{v_1} = C_{A1}(1-\alpha)$$

$$= C_{A0}(1-\alpha)$$

Now, we also need various other things to be able to put the process equations in the form that we can solve. So, I have just put them down, just to put it in the context; v 1, we just now said is v 0, divided by 1 minus of y times 1 minus of alpha. Similarly, what is C b 2? Concentration component 2 is F b 2 divided by v 2. F b 2, we have said, based on our understanding of the stoichiometry of reaction is F b 2. What is adjust position 2, is simply, whatever reacts F a 1 times alpha is F b 2.

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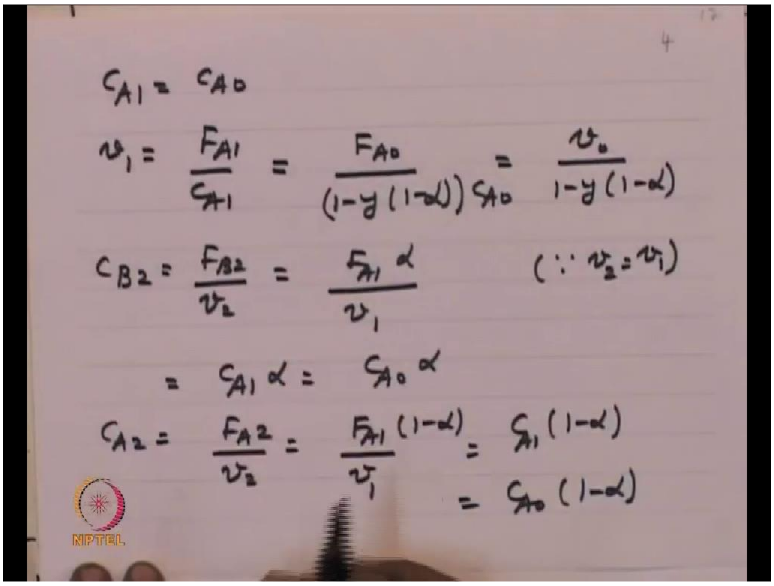

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$$C_{A1} = C_{A0}$$

$$v_1 = \frac{F_{A1}}{C_{A1}} = \frac{F_{A0}}{(1-y(1-\alpha))C_{A0}} = \frac{v_0}{1-y(1-\alpha)}$$

$$C_{B2} = \frac{F_{B2}}{v_2} = \frac{F_{A1}\alpha}{v_1} \qquad (\because v_2 = v_1)$$

$$= C_{A1}\alpha = C_{A0}\alpha$$

$$C_{A2} = \frac{F_{A2}}{v_2} = \frac{F_{A1}(1-\alpha)}{v_1} = C_{A1}(1-\alpha)$$

$$= C_{A0}(1-\alpha)$$

So, it is what is mentioned here; F a 1 times alpha is F b 2. What is the volumetric flow? This particular reaction A goes to B; there is no volume change; therefore, whatever is volumetric flow at position 1; we should expect that be the volumetric position 2, because there is no volume change at the reaction. Therefore, v 2 equal to v 1. Therefore, C b 2 becomes C a 1 times alpha, and we have said just now that C a 1 is, because C a stream 5 is made up to concentration of 100 cubic kg per cubic meters, same as C a 0. There will be position 1; concentration C a 0. So, we replace C a 1 as C a 0. Therefore, we get C b 2 as C a 0 times alpha. What is C a 2? C a 2 is F a 2 by v 2, which is F a 1, 1 minus alpha v 1; once again, it is C a 0, 1 minus alpha. Notice that our effort is to put every variable of interest, in terms of parameters process variables which, we are interested in, so that, we can do our optimization properly.

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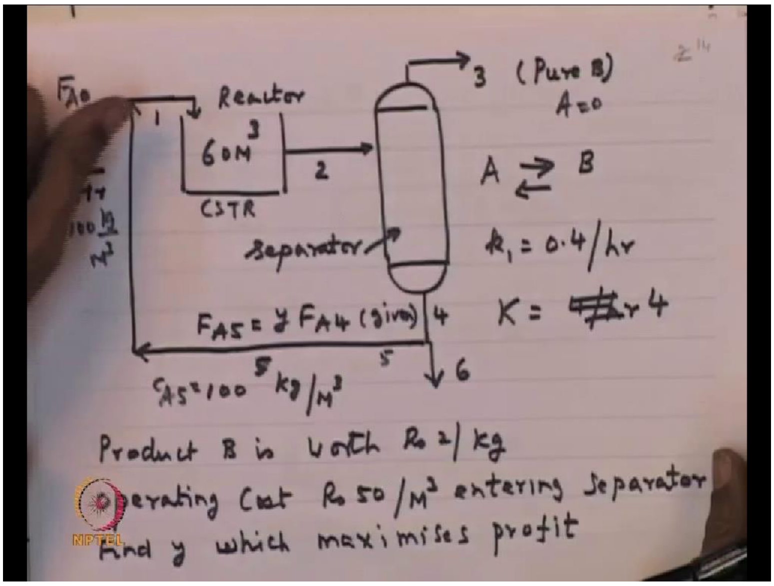

Product B is worth Rs 2/kg

Operating Cost Rs 50/M^3 entering separator

Find y which maximises profit

What we have done so far is that we have expressed concentrations at position 1, concentrations at position 2, volumetric flow at position 1, volumetric flow at position 2; that means, whatever affects the process, the reactor; all that we have expressed in terms of alpha and y. Therefore, we are now in a position to write the design equation for this reaction equipment, so that, we can understand how they come together to affect the process. So, this is what is written here. It says, CSTR equation says that the volume of CSTR is F a 1 times alpha, divided by the rate at which, the reaction occurs at position 2.

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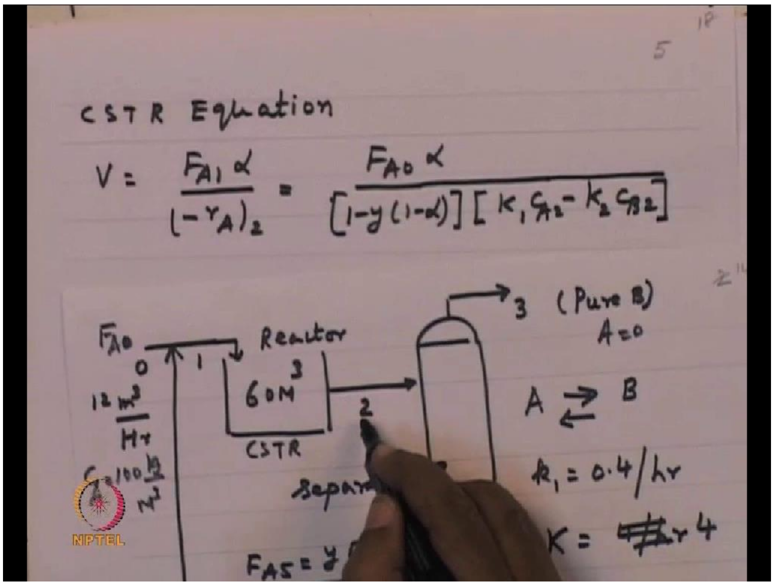
CSTR Equation

$$V = \frac{F_{A1}\,\alpha}{(-r_A)_2} = \frac{F_{A0}\,\alpha}{[1-y(1-\alpha)][k_1 C_{A2} - k_2 C_{B2}]}$$

Notice here that CSTR operates at exit concentration, which is position 2. That is how it is written, r a at position 2. Therefore, whenever we write the reaction rate expressions at position 2, we should take the concentrations at position 2 to write our rate expressions. That is what we have done here.

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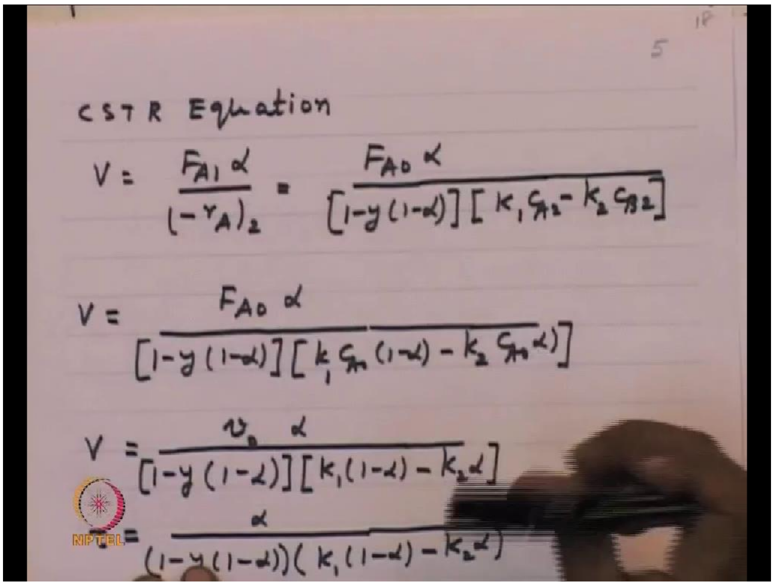

CSTR Equation

$$V = \frac{F_{A1}\alpha}{(-r_A)_2} = \frac{F_{A0}\alpha}{[1-y(1-\alpha)][k_1 C_{A2} - k_2 C_{B2}]}$$

$$V = \frac{F_{A0}\alpha}{[1-y(1-\alpha)][k_1 C_{A0}(1-\alpha) - k_2 C_{A0}\alpha)]}$$

$$V = \frac{v_0 \alpha}{[1-y(1-\alpha)][k_1(1-\alpha) - k_2\alpha]}$$

$$= \frac{\alpha}{(1-y(1-\alpha))(k_1(1-\alpha) - k_2\alpha)}$$

So, F a 1 times alpha, we have already shown that F a 1 is, this, we have shown that F a 1 is F a 0 times 1 minus y times 1 minus alpha.

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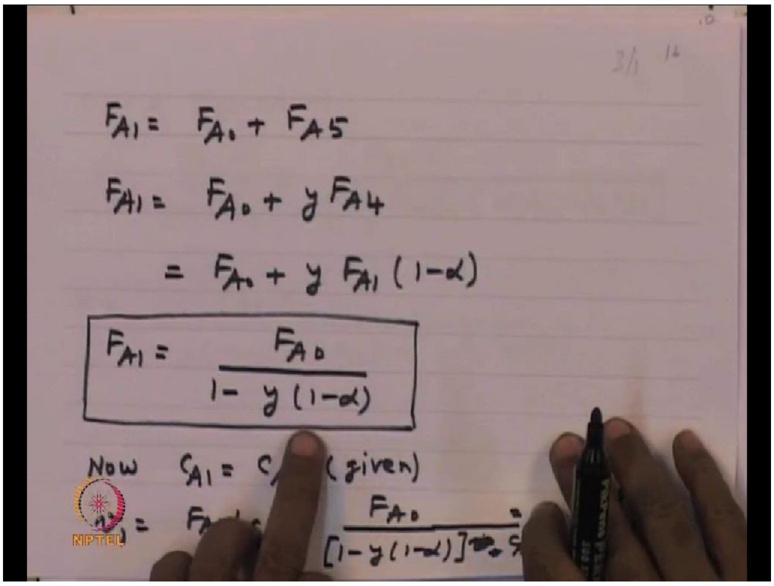

$$F_{A1} = F_{A0} + F_{A5}$$

$$F_{A1} = F_{A0} + y F_{A4}$$

$$= F_{A0} + y F_{A1}(1-\alpha)$$

$$\boxed{F_{A1} = \frac{F_{A0}}{1-y(1-\alpha)}}$$

Now $C_{A1} = C$ (given)

$$= \frac{F_{A0}}{[1-y(1-\alpha)]}$$

So, you have replaced F a 1 in terms of F a 0, divided by 1 minus of alpha and what is r a 2; minus of r a 2 is a rate of chemical reaction. So, r a 2 is mentioned here. So, it is K 1 C a 2 minus of K 2 C b 2 rate at which, this reaction is taking place with a minus sign is given by this, because r a; we all know this; r a by definition, is K 2 C b 2 minus of K 1 C a 2.

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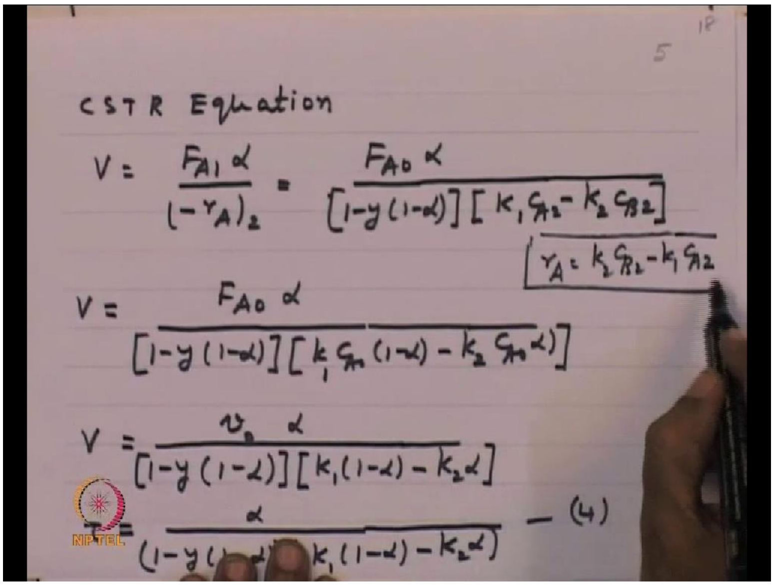

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CSTR Equation

$$V = \frac{F_{A1}\,\alpha}{(-r_A)_2} = \frac{F_{A0}\,\alpha}{[1-y(1-\alpha)][k_1 C_{A2} - k_2 C_{B2}]}$$

$$\boxed{r_A = k_2 C_{B2} - k_1 C_{A2}}$$

$$V = \frac{F_{A0}\,\alpha}{[1-y(1-\alpha)][k_1 C_{A0}(1-\alpha) - k_2 C_{A0}\alpha)]}$$

$$V = \frac{v_0\,\alpha}{[1-y(1-\alpha)][k_1(1-\alpha) - k_2\alpha]}$$

$$\tau = \frac{\alpha}{(1-y(\quad k_1(1-\alpha) - k_2\alpha)} \quad -(4)$$

This is something that we all know that the first order reaction that is given, takes place. Then, this is the rate function, which will account for. So, what we have done now? We have replaced r a in terms of K 1, C a 2 minus of K 2, C b 2; this subscript 2 refers to position 2 where K 1 and K 2 refers to these reactions.

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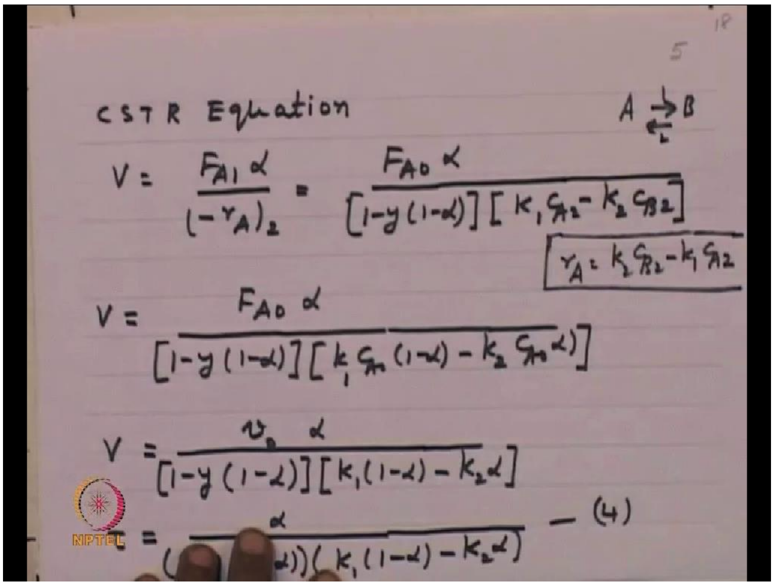

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5

CSTR Equation

$$A \underset{2}{\overset{1}{\rightleftarrows}} B$$

$$V = \frac{F_{A1}\,\alpha}{(-r_A)_2} = \frac{F_{A0}\,\alpha}{[1-y(1-\alpha)][k_1 C_{A2} - k_2 C_{B2}]}$$

$$\boxed{r_A = k_2 C_{B2} - k_1 C_{A2}}$$

$$V = \frac{F_{A0}\,\alpha}{[1-y(1-\alpha)][k_1 C_{A0}(1-\alpha) - k_2 C_{A0}\alpha)]}$$

$$V = \frac{v_0\,\alpha}{[1-y(1-\alpha)][k_1(1-\alpha) - k_2\alpha]}$$

$$\tau = \frac{\alpha}{(\quad \alpha))(k_1(1-\alpha) - k_2\alpha)} \quad -(4)$$

This reaction A going to B; this is reaction 1 and B going to A; this is reaction 2. So, we have the size of the CSTR or size of the stirred tank, is now, given in terms of F a 0 alpha, divided by our parameters, y and alpha, which define the process. So, we can see once again, we are able to put everything in terms of the parameters of our interest. So, we can manipulate and simplify this, and we get residence time in the reaction equipment, is given by this relationship; alpha divided by y, minus of y times from minus of alpha, multiplied by the rate function, appropriately modified. So, you have an equation now. Basically, what we have done; we have set up an equation for the chemical reactor, which takes into account, the inputs and outputs are appropriately, and that final form of that expression, which relates residence time in terms of parameters, which we are interested in. Our parameters are alpha and y; see, that is how it, you know, the whole balances, help us to do.

Now, we said just a little while ago that whenever, we have this kind of recycles, there is an optima that exists, because of cost; cost of operation and cost benefits of producing the product.

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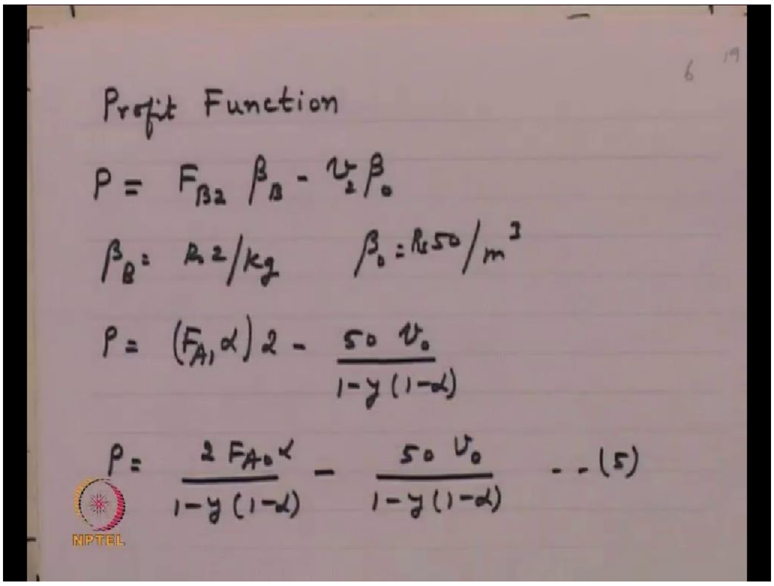

Profit Function

$$P = F_{B2}\beta_B - v_2\beta_0$$

β_B = Rs 2/kg $\quad \beta_0$ = Rs 50/m^3

$$P = (F_{A1}\alpha)2 - \frac{50\,v_0}{1-y(1-\alpha)}$$

$$P = \frac{2F_{A0}\alpha}{1-y(1-\alpha)} - \frac{50\,v_0}{1-y(1-\alpha)} \quad \text{--(5)}$$

So, we will see in the optima and in this particular exercise, cost functions are also given. For example, in this particular problem, it is specified that the profit that you are likely to get from this process, is the amount of product F b 2 that we make, multiplied by the worth of that product, which is beta b, is the worth of the product. So, this is the benefit of doing this process. What is the cost of running the process? It is given as it is equal to the material that is entering the separator; that means, volumetric flow entering the separator, multiplied by the cost per cubic meter of solution, entering the separator. What is the cost of operating this process? It says it is equal to v 2; v 2 is volumetric flow here, multiplied by beta 0, while beta 0 is the cost of operation of this process; X plus per cubic meter of solution, entering the separator. This is what is given.

Now, we have this cost function, the profit function F b 2 times beta b and minus of v 2 times beta; not both are given; beta naught is given; beta b is given. Therefore, we have now, a cost, a profit function, which very nicely, stated and we notice once again, that F b 2 is F a 1 alpha while, v 2 is v 1.

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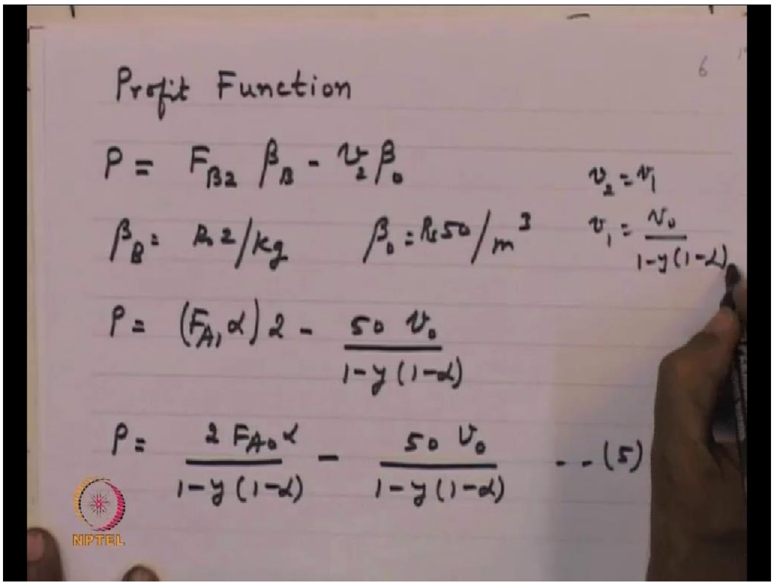

Profit Function

$$P = F_{B2}\,\beta_B - v_2\,\beta_0 \qquad v_2 = v_1$$

$$\beta_B : Rs\ 2/kg \qquad \beta_0 : Rs\ 50/m^3 \qquad v_1 = \frac{v_0}{1-y(1-\alpha)}$$

$$P = (F_{A1}\alpha)\,2 - \frac{50\,v_0}{1-y(1-\alpha)}$$

$$P = \frac{2F_{A0}\alpha}{1-y(1-\alpha)} - \frac{50\,v_0}{1-y(1-\alpha)} \quad \text{..(5)}$$

We know v 2 is v 1; we have already mentioned that v 2 is v 1, and v 1 is in terms of v 0; we already done that 1 minus of y times 1 minus alpha; we know all that.

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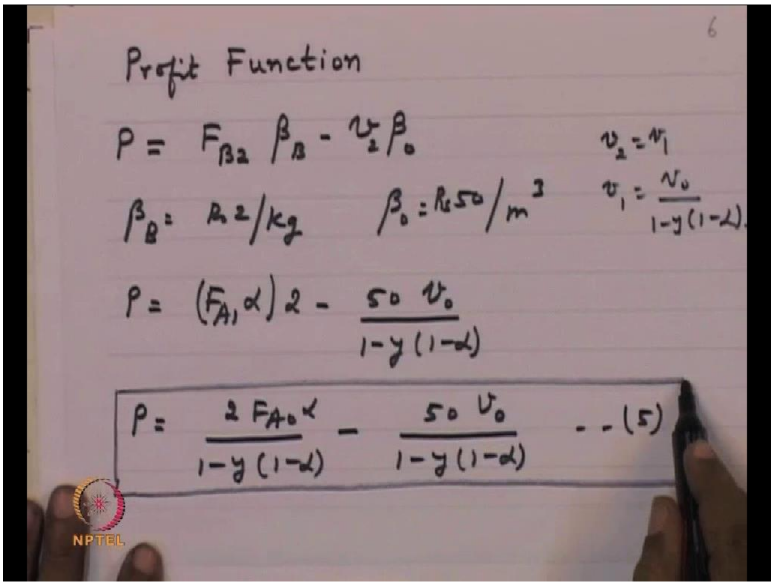

Profit Function

$$P = F_{B2}\,\beta_B - v_2\,\beta_0 \qquad v_2 = v_1$$

$$\beta_B : Rs\ 2/kg \qquad \beta_0 : Rs\ 50/m^3 \qquad v_1 = \frac{v_0}{1-y(1-\alpha)}$$

$$P = (F_{A1}\alpha)\,2 - \frac{50\,v_0}{1-y(1-\alpha)}$$

$$\boxed{P = \frac{2F_{A0}\alpha}{1-y(1-\alpha)} - \frac{50\,v_0}{1-y(1-\alpha)} \quad \text{..(5)}}$$

So, we can replace everything in terms of numbers that you know, in terms of parameter that you know, so that, we finally, end up with an equation that defines the profit, that you will get from this process. Once again, this profit function is in terms of two parameters, y and alpha. So, we are calling what we have sent so far. We have done a little earlier and we calling once again, that what we have done so far. Just quickly recap, because important to understand why we are doing this.

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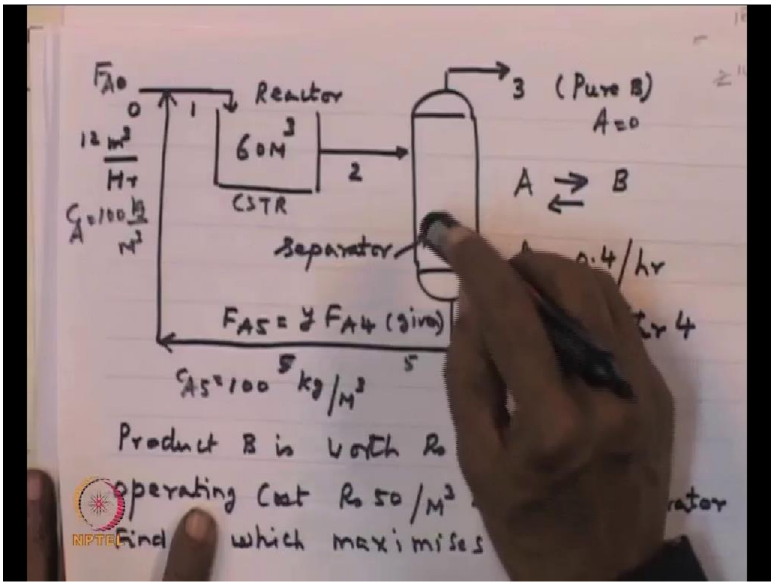

We have a reactor, we have a separator. Now, the fact that the reactor and separator interplay and there is an optimum value at which, the process if it operates, then the benefits are the highest. To quantitate this, this problem has been taken. So, what we have done, first done, is that we have done a balance for the CSTR and that balance told us that the residence time is related to alpha and y by this relation equation 4.

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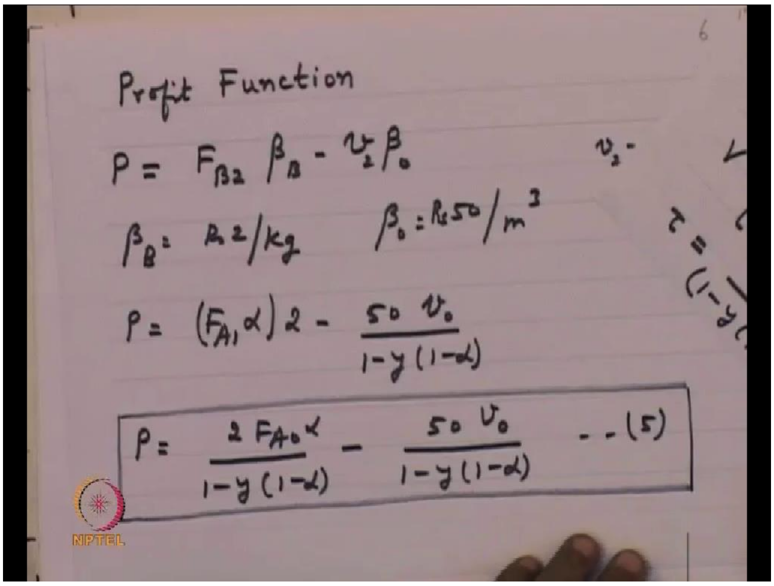
Profit Function

$P = F_{B2}\beta_B - v_2\beta_0$ $v_2 =$

$\beta_B = Rs\ 2/kg$ $\beta_0 = Rs\ 50/m^3$

$P = (F_{A1}\alpha)2 - \frac{50\, v_0}{1-y(1-\alpha)}$

$$\boxed{P = \frac{2F_{A0}\alpha}{1-y(1-\alpha)} - \frac{50\, v_0}{1-y(1-\alpha)} \quad \text{--}(5)}$$

Now, then, next thing what we did is that we have set up a profit function, which says us a profit depends upon alpha and y as per equation 5. Your equation 4, which relates to the process; equation 5, which relates to the cost or profit; therefore, now you have to only manipulate equation 4 and 5 to see how we can handle the whole issue. Interestingly, if you look at equation 5, we find that this term 1 minus of y times 1 minus alpha appears. At the same time, look at equation 4; this term 1 minus of y times 1 minus of alpha appears. On other words, it is possible for us to find out the value of 1 minus of y times 1 minus of alpha from equation 4, and then substitute in equation 5. The interesting thing is that the moment we do that, y disappears from our formulation. So, moment we replace the term 1 minus of y time 1 minus of alpha from equation 4 into equation 5; that is what I have tried to do here; from equation 4 here, I have expressed it in terms of alpha and tau and others.

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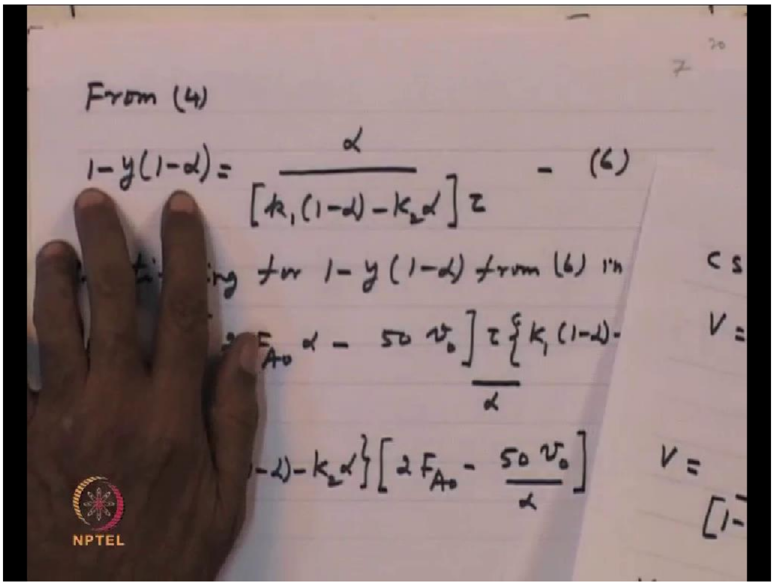

From (4)

$1-y(1-\alpha) = \dfrac{\alpha}{[k_1(1-\alpha)-k_2\alpha]\tau}$ - (6)

ing for $1-y(1-\alpha)$ from (6) in

$F_{A0}\alpha - 50 v_0]\dfrac{\tau\{k_1(1-\alpha)-}{\alpha}$

$-\alpha)-k_2\alpha\}[2F_{A0} - \dfrac{50 v_0}{\alpha}]$

C s

V =

V =

[1-

So, you find here, 1 minus of y times 1 minus of alpha now, depend only an alpha and tau; tau is a process variable, which in this case, is specified by the problem statement. So, what we have been able to do is that by appropriately, formulating the problem in our hand; you are able to eliminate one of the two parameters, which is y, so that, you are able to get everything in terms of one variable, which is alpha. So, by substituting for this term 1 minus of y times 1 minus of alpha, which is equation 6 into equation 5; what is the equation 5? Our equation 5 is a profit function.

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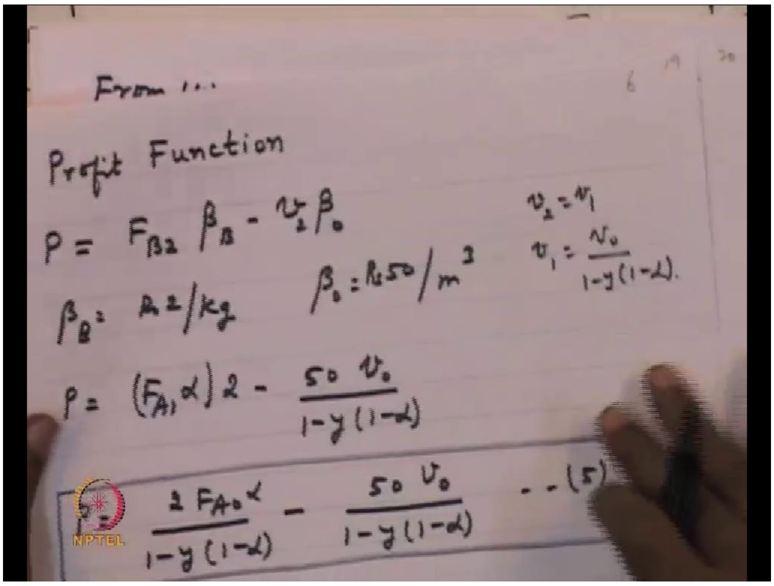

6

From ...

Profit Function

$P = F_{B2}\,\beta_B - v_2\,\beta_0$ $\qquad v_2 = v_1$

$\beta_B = Rs\ 2/kg \qquad \beta_0 = Rs\ 50/m^3 \qquad v_1 = \frac{v_0}{1-y(1-\alpha)}.$

$$P = (F_{A1}\alpha)\,2 - \frac{50\,v_0}{1-y(1-\alpha)}$$

$$\boxed{\frac{2F_{A0}\alpha}{1-y(1-\alpha)} - \frac{50\,v_0}{1-y(1-\alpha)}} \quad \ldots(5)$$

Now, you are able to get the profit function, the whole profit function.

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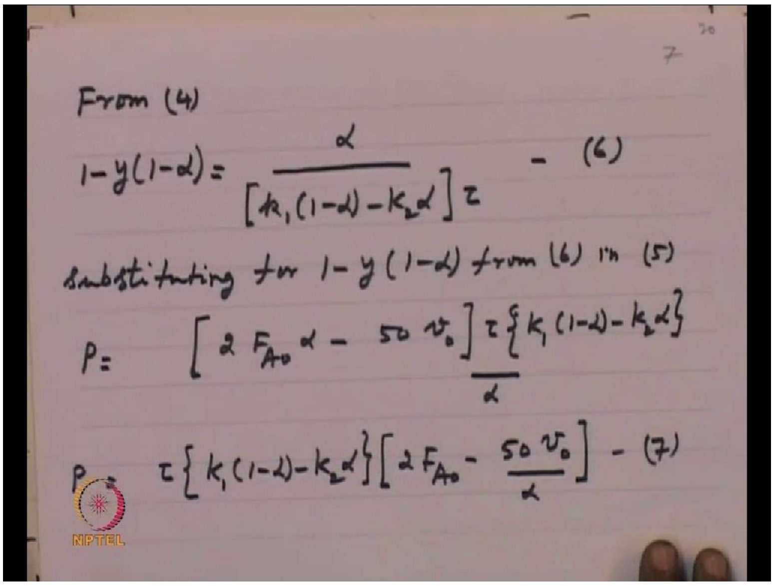

7

From (4)

$$1-y(1-\alpha) = \frac{\alpha}{[k_1(1-\alpha)-k_2\alpha]\,\tau} \quad -(6)$$

substituting for $1-y(1-\alpha)$ from (6) in (5)

$$P = [2F_{A0}\alpha - 50\,v_0]\,\frac{\tau\{k_1(1-\alpha)-k_2\alpha\}}{\alpha}$$

$$P = \tau\{k_1(1-\alpha)-k_2\alpha\}\left[2F_{A0} - \frac{50\,v_0}{\alpha}\right] \quad -(7)$$

If you eliminate this term 1 minus of y times 1 minus of alpha, the profit function now, looks like this, which is essentially, a function of alpha. So, now, what we have done we had we had a problem in which, there are two parameters, y and alpha, which determined the process. Through the design equation for the CSTR, we could knock out one of them. Therefore, your profit function now, depends only an alpha. Now, the question, problem statement is that find the value of y, which maximizes the operational profit of the plant; that is the question that we have to solve. So, what we have done? We have now eliminated y, but the question is what is the value of y, which maximizes p; that is the question. But what we have done is that we have eliminated y; we have an equation which represents p in terms of alpha. We are able to maximize profit with alpha as our variable. So, we have to now, show the maximizing p with respect to alpha, is same as maximizing p, with respect to y.

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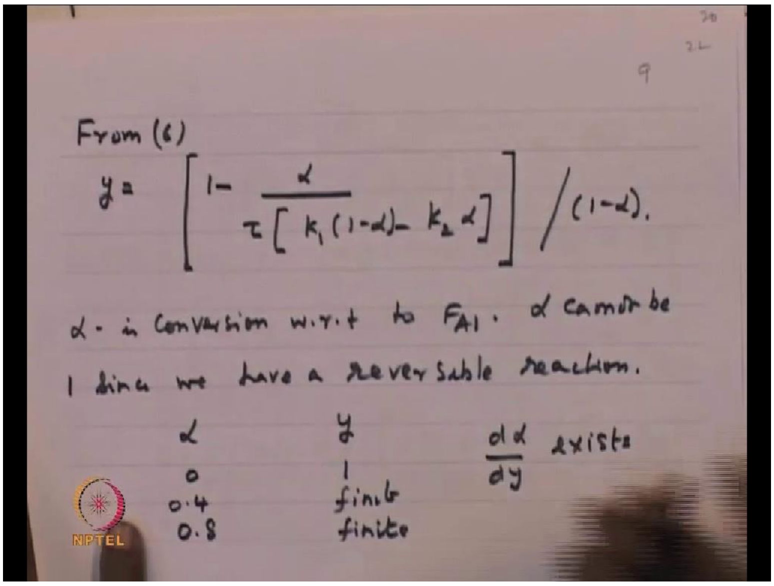

9

From (6)

$$y = \left[1 - \frac{\alpha}{\tau\left[k_1(1-\alpha) - k_2\alpha\right]}\right] / (1-\alpha).$$

α - is Conversion w.r.t to F_{A1}. α cannot be 1 since we have a reversable reaction.

α	y
0	1
0.4	finite
0.8	finite

$\frac{d\alpha}{dy}$ exists

Now, to do this; this is not very difficult to do, but to do this, we have equation 6 which, we already set up. We have already set up equation 6 as you all know. So, from this equation, we can express y in terms of alpha. So, I have done this here. So, I have done y in terms of alpha.

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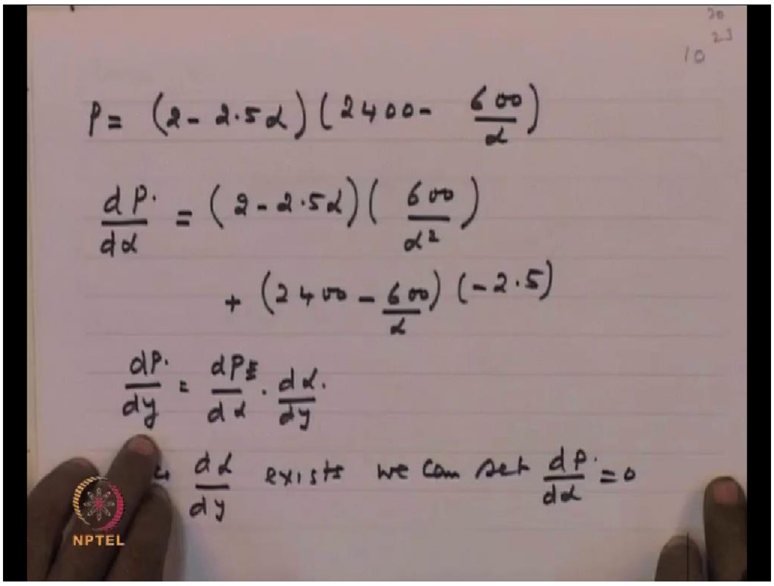

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$$P = (2 - 2.5\alpha)\left(2400 - \frac{600}{\alpha}\right)$$

$$\frac{dP}{d\alpha} = (2 - 2.5\alpha)\left(\frac{600}{\alpha^2}\right) + \left(2400 - \frac{600}{\alpha}\right)(-2.5)$$

$$\frac{dP}{dy} = \frac{dP}{d\alpha} \cdot \frac{d\alpha}{dy}$$

$\frac{d\alpha}{dy}$ exists we can set $\frac{dP}{d\alpha} = 0$

Now, if we do d alpha, let us say, we have to show that dp dy; I have written it here, see, we have to do dp dy is same as dp d alpha, because d alpha dy is finite. Since, d alpha dy is finite, if we maximize p with respect to alpha, it is same as maximizing p with respect to y. I hope it is clear. Let me run through this, once again. We spend a lot of time so far, trying to express our process in terms of y and alpha. Then, we eliminated y and got the whole profit function in terms of alpha; we have done that here by putting all the numbers appropriate to the process. Now, the question remains is that is the maxima of p or the profit in term with respect to y, same as the maxima with respect to alpha? The answer is that if d alpha by dy is finite in the region of our interest, which it is in this case; you can check for yourself. Therefore, dp dy is same as dp d alpha, equal to 0. So, if you put dp dy d alpha equal to 0, the point of maxima that you will get is also the same point of maxima, corresponding to dp dy. So, what are we trying to say? What we are trying to say is that if we simply, maximize p with respect to alpha, it is as good as maximizing p with respect to y. So, what have we done here? You do dp d alpha. When you do dp d alpha, what do we get?

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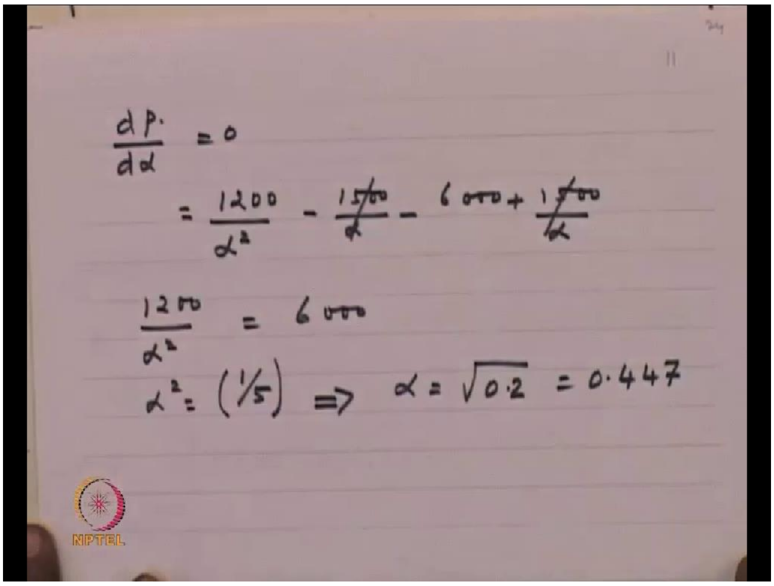

$$\frac{dp}{d\alpha} = 0$$

$$= \frac{1200}{\alpha^2} - \cancel{\frac{1500}{\alpha}} - 6000 + \cancel{\frac{1500}{\alpha}}$$

$$\frac{1200}{\alpha^2} = 6000$$

$$\alpha^2 = \left(1/5\right) \Rightarrow \alpha = \sqrt{0.2} = 0.447$$

When you do dp d alpha, we find that the value of alpha at which, p takes the, p is maxima; counts out to be 0.447.

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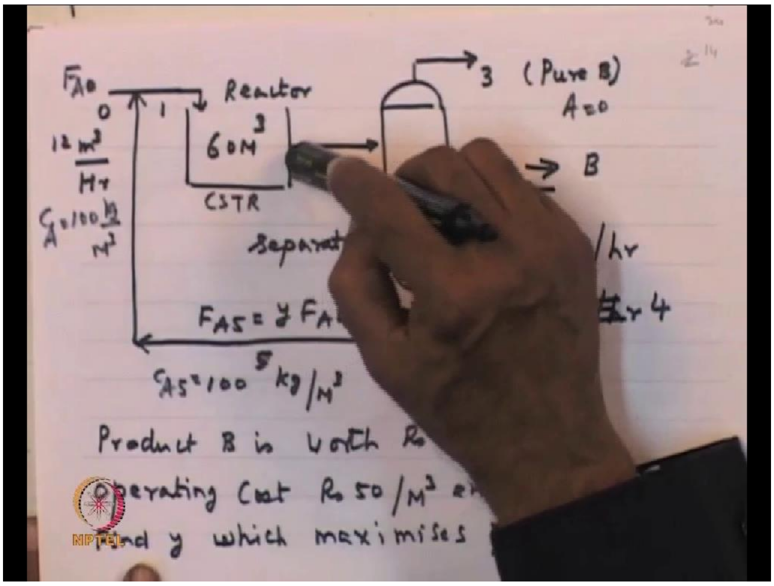

Product B is worth Rs

Operating Cost Rs 50/M^3

nd y which maximises

On other words, what we are saying is that in this process, the value of alpha; alpha is the fraction of a F a 1, which is converted. It is 0.447. If you operate at that value of alpha, then this whole process, the profit of this process meets the highest. So, that is what we have been able to conclude by looking at this process. Now, the question that is being asked is given that value of alpha is 0.447, what is the conversion that we can expect from this process, and what is the value of y that we can get from this process? What is the fraction; y is what; is the fraction; y is a fraction of stream 4 which, you have to recycle. We still do not know y; you only know alpha. How do you find y?

Y, we can find from our equation 6.

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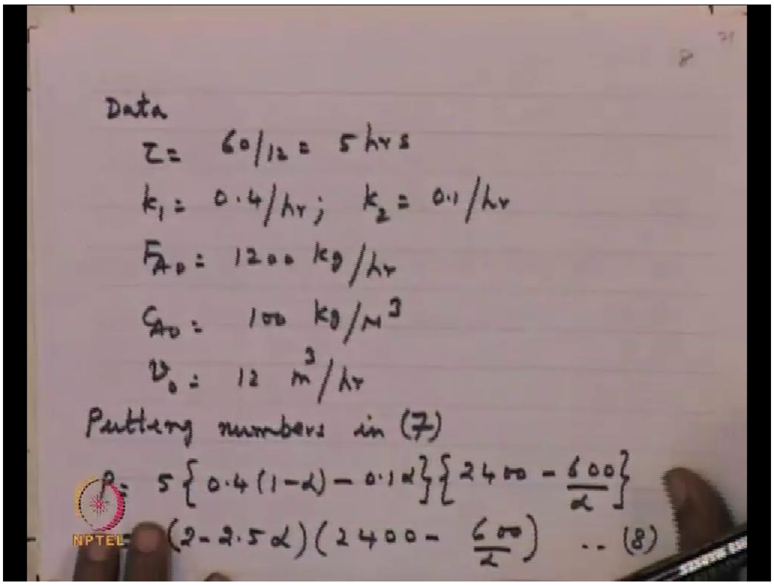

Data

$\tau = 60/12 = 5\ hrs$

$k_1 = 0.4/hr;\ k_2 = 0.1/hr$

$F_{A0} = 1200\ kg/hr$

$C_{A0} = 100\ kg/m^3$

$v_0 = 12\ m^3/hr$

Putting numbers in (7)

$$P = 5\{0.4(1-\alpha) - 0.1\alpha\}\left\{2400 - \frac{600}{\alpha}\right\}$$

$$= (2-2.5\alpha)\left(2400 - \frac{600}{\alpha}\right) \quad ..\ (8)$$

If equation 6, if you know alpha, you can find y, because this is equation 6 and in this process, all the numbers are specified. You can see here; tau is given as 5 hours; k 1 is given as 0.4; k 2 is given as 0.1; F a 0 is given as 1200; C a 0 is given; v naught is given. Therefore, you can get the value of y from this equation. So, you can put your numbers and see how it looks. I have done that, and then it turns out that y is 0.89.

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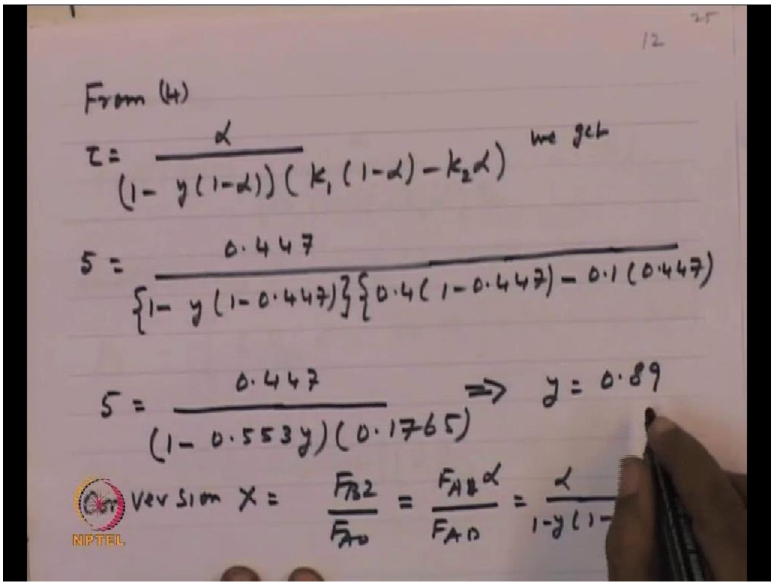

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12

From (4)

$$\tau = \frac{\alpha}{(1-y(1-\alpha))(k_1(1-\alpha)-k_2\alpha)} \quad \text{we get}$$

$$5 = \frac{0.447}{\{1-y(1-0.447)\}\{0.4(1-0.447)-0.1(0.447)\}}$$

$$5 = \frac{0.447}{(1-0.553y)(0.1765)} \Rightarrow y = 0.89$$

Conversion $X = \frac{F_{B2}}{F_{A0}} = \frac{F_{A1}\alpha}{F_{A0}} = \frac{\alpha}{1-y(1-}$

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This is the number y; that is 0.89. So, what are we getting? Now, if you know alpha is 0.447; y is 0.89. Now, if I ask you what is a conversion that we can get from this process; how is conversion defined? Conversion is defined as the amount of product that you make, divided by amount of feed that you put into the process. So, how much product have we made, is F a 1 times alpha. How much of feed have you put in; it is F a 0 and what is F a 1? F a 1 is 1 by 1 minus of F a 1; F a 1 is F a 0, divided by this; F a 0 gets cancelled. Therefore, this conversion that you will expect from this process is alpha, divided by 1 minus of y times 1 minus of alpha. If you put here numbers, alpha is 0.447 and therefore, y is 0.89; you put all the numbers. You will get, the conversion to be expected in this process, is 0.88.

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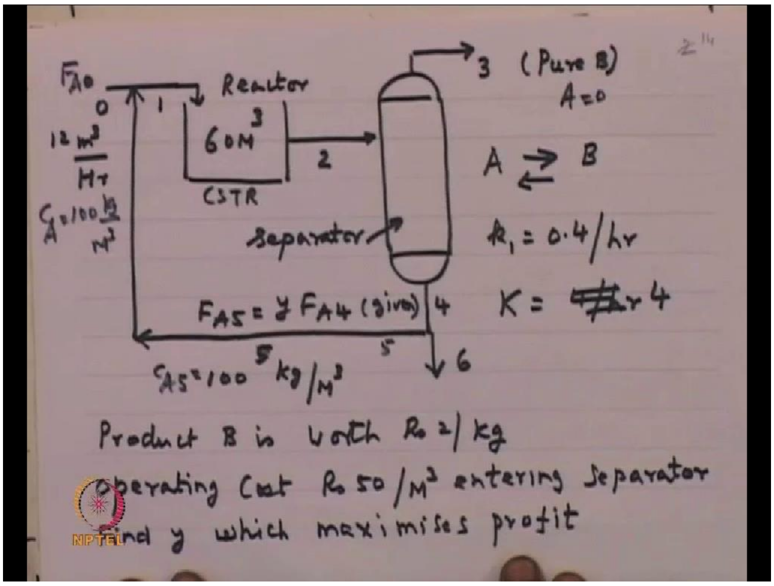

Product B is worth Rs 2/kg

Operating Cost Rs 50/M^3 entering Separator

nd y which maximises profit

So, just to put this in the context, the context is important that if you have a process in which, you have continuously processing in a reaction equipment, CSTR, and then you are removing the product in a separator, and then you are recycling only a part of it, because that is operationally more profitable. The fraction y that maximizes the profit of this plant is coming out of this formulation that I have discussed with you, just now. So, depending upon the worth of this product and the operating cost, how these two come together; if they change, of course, the value of alpha will change. Therefore, value of y will change and therefore, the conversion from the plant will also change. So, these numbers essentially, determine at what point, you must operate the process. So, this is what we have try to get across in this exercise of recycle effects in the process. Now, before we conclude, let me just draw your attention to one more issue, regarding autocatalytic reactions.

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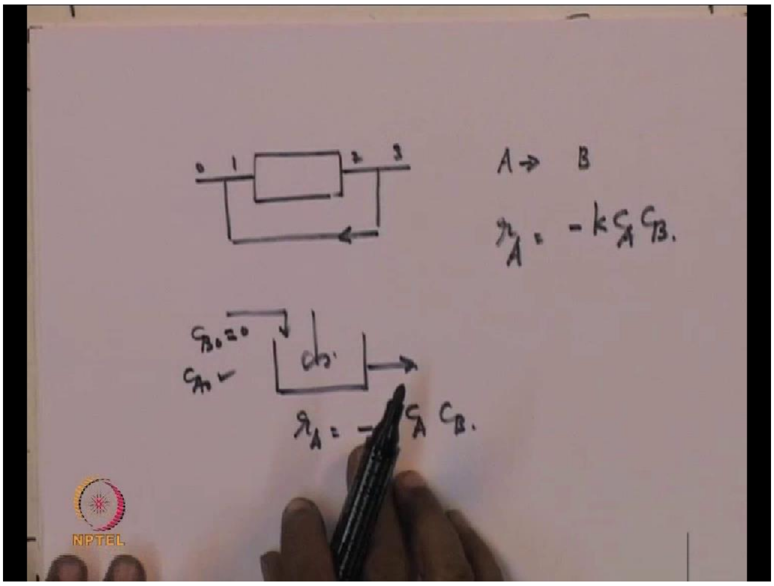

When we have an autocatalytic reaction A going to B and r a is minus of k times C a and C b; we said that if this reactor is a stirred tank, which means, comes in and goes out, then r a is minus of k times C a and C b. Then, it is not necessary to have C b 0; C b zero can be C a; C a 0 is finite, but C b 0 can be 0 even, then the reaction will proceed. We have explained this last time when we met. When we said, this is because in this, when you look at the unsteady state during the start up, as long as during start up, you have put in some C b into the process, then stirred tank remembers that start up addition of C b and therefore, that process will be able to get initiated, because of the presence of, even, traces of C b in the equipment.

On other words, the stirred tank is an instance of a reaction equipment where, you do not need feed, sorry, product to be primed into the feed, as for an autocatalytic reaction, but if the same thing is to be done in a PFR, without recycle; if you have to do in a PFR, same autocatalytic reaction, because there is no mixing here and therefore, the feed does not contain product.

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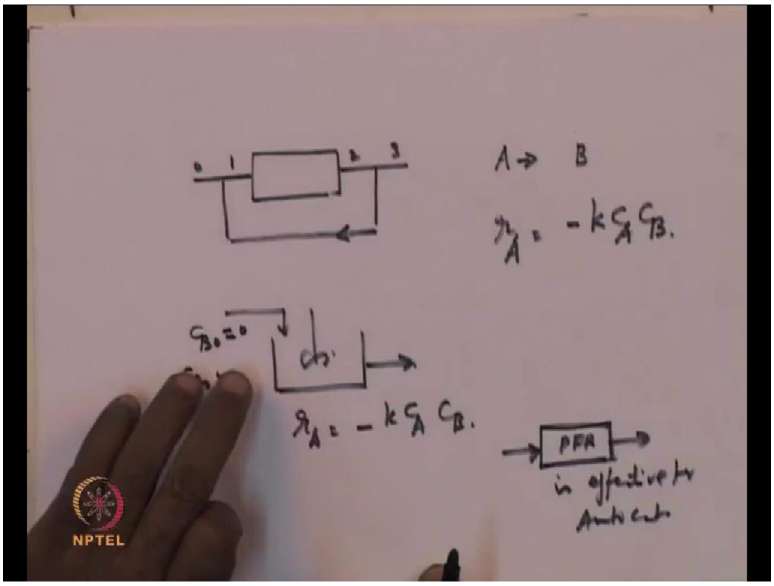

Therefore, you will find the reaction will not take off. So, PFR is not effective for autocatalytic reaction.

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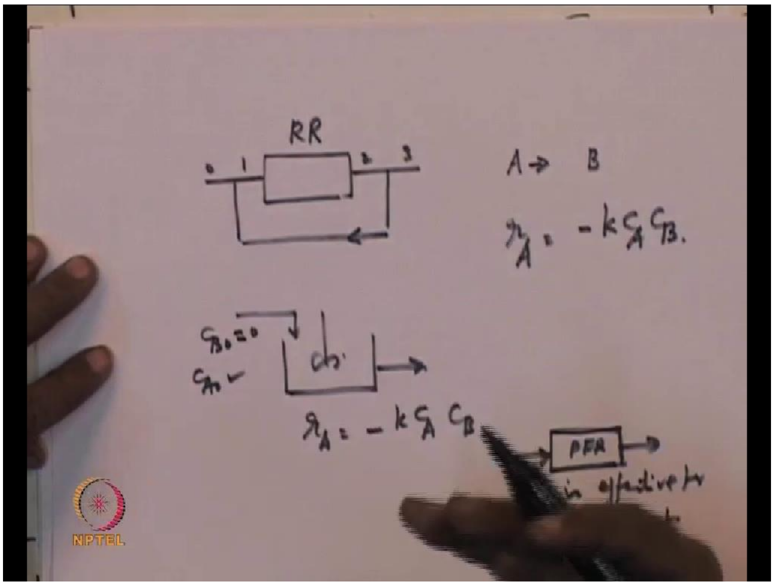

CSTR and recycle reactors are extremely, valuable for autocatalytic reaction, because you are able to; in the recycle reactor, this is a recycle reactor; you are able to recycle the product and therefore, the reaction gets initiated. Therefore, this is very valuable from the point of view of autocatalytic reactions. Stirred tank; since, the recycle, because of recycle, because of infinite recycle; that is what we have understood; this, we find is very effective from the point of view of autocatalytic reactions.

I will stop this with this process.