Advanced chemical Reaction Engineering
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Lecture - 08
Multiple Reactions – II

We get started with multiple reactions. We have already shown the following result.

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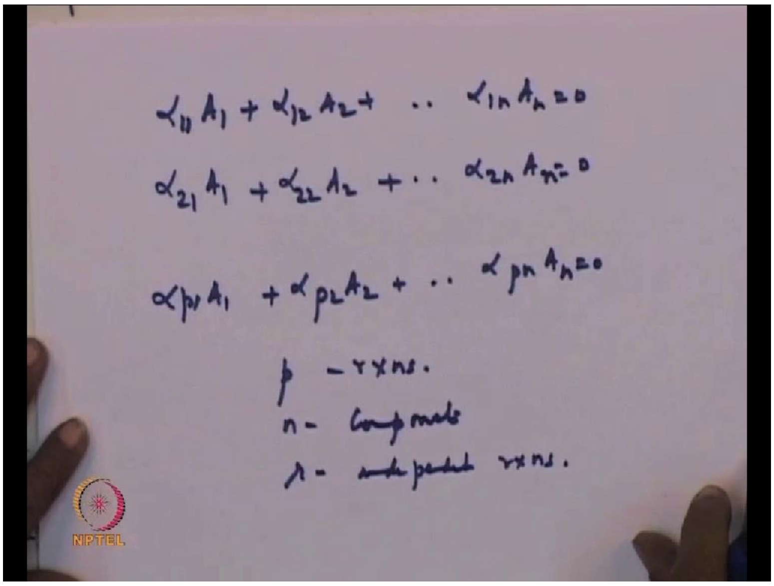

Let us quickly, state that result that if we have a multiple reaction like alpha 1 1, a 1 plus alpha 1 2, a 2; alpha 1 n, a n equal to 0; alpha 2 1, a 1, alpha 2 2, a 2, 2 n a n equal to 0; alpha p 1 p 2, a 2, alpha p n, a n. So, there are p reactions; p rate processes; n components and r independent reactions. When we said independent reactions, what we meant is that this system requires r quantities to be specified to be able to characterize the system, as it changes in the course of the reaction. What we want to do now, is take one example, and then understand what we have done so far.

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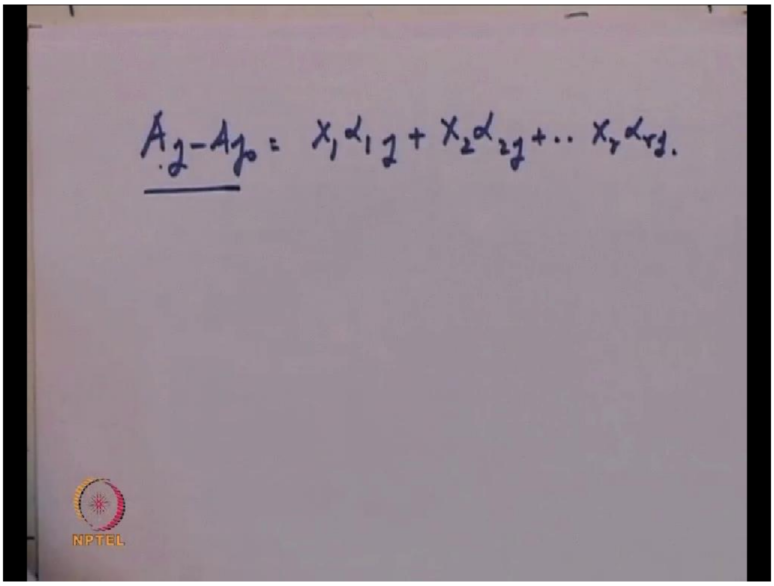

So, to write the stoichiometry, we said we can write a j minus of a j 0 can be given as x 1 alpha 1 j, x 2 alpha 2 j, up to x r alpha r j. Sometimes, we normalise it with respect to a reference, in which case, each of these x's have no dimensions. If we do not normalize, each of them will have the same units as a j, depending upon how we do the exercise. Based on this, we are able to write the design equations for various equipments, including (( )), CSTR and so on. Now, we will take an example to see how to make use of this result in our designs.

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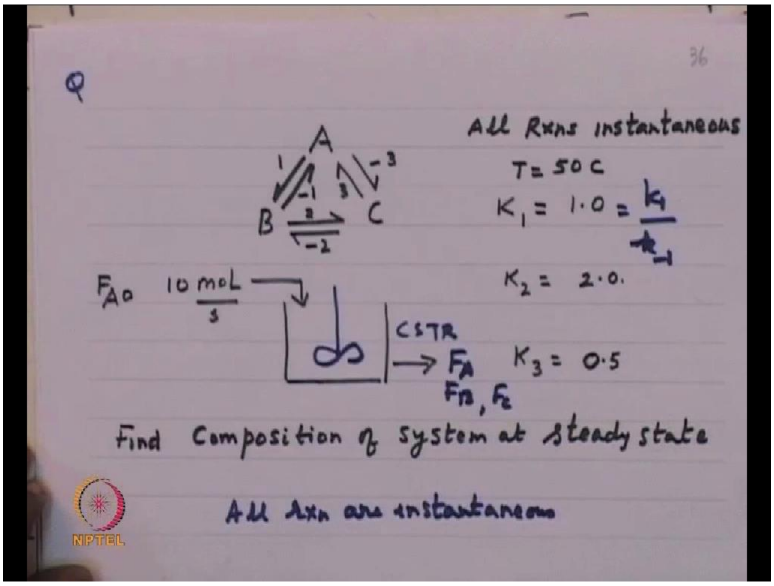

For that, what we have is yes, this is a multiple reaction; A goes to B; B goes to C and C goes to A. So, I have written 1 and minus 1, showing that forward and backward reactions, and we are trying to do this in a stirred vessel or a CSTR, and some numbers are given; k 1, k 1 is simply, k 1 by k, sorry, k minus 1. Similarly, k 2 and k 3; all reactions are instantaneous. If A enters at this rate, what is the composition here? What is F a, F b and F c; this is what we want to calculate. We want to use this procedure plus, we also want to use procedures which, we think are common sense, and see how best all these procedures come together.

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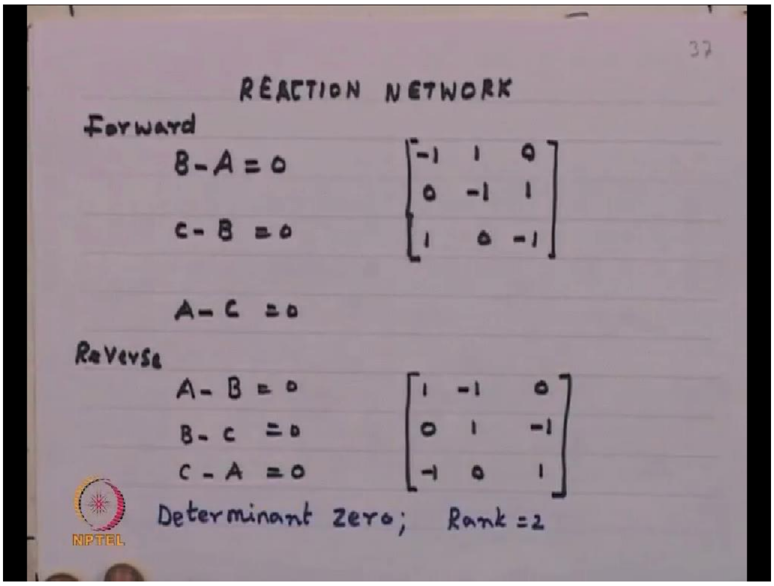

Now, to do this what we normally, do is the following. Suppose these reactions were not reversible; A goes to B; B goes to C; C goes to A; assuming that not reversible; that means, there are only three reaction sets, which is written in this form; B minus A equal to 0; C minus B equal to 0; A minus C equal to 0; assuming that they are not reversible. Then, the matrix we works, called as the sticheometry matrix, looks like this. Now, if you take only the reverse reaction, then the sticheometry matrix look like this; is this clear, what we are saying? We have only, A goes to B; B goes to C; C goes to A; assuming this is not reversible. Then, this is the reaction. This is the sticheometry matrix. If only the reverse reaction is occurring; that means, B goes to A; C goes to B; A goes to C; then, this is the sticheometry matrix.

Now, we can actually, do the determinant and find out for ourselves, in very simple determinant; we can do it right now. Find out the rank of this matrix, please. Find the rank of this matrix; minus 1 multiplied by this, please. Find the rank. Just, we have to see, what is the determinant. Find the determinant of this matrix, will tell you it is 0. You can just expand that and find out yourself, the determinant is 0, all right, which means that this matrix is a singular, showing that all the three reactions are not independent. Only if we take any second order matrix; for example, any two, we see it is independent. So, showing that there are two reactions are independent; is this clear, how to find out? Now, you can combine forward reaction and backward reaction and write the much bigger matrix and also, try to see what is the rank of this matrix?

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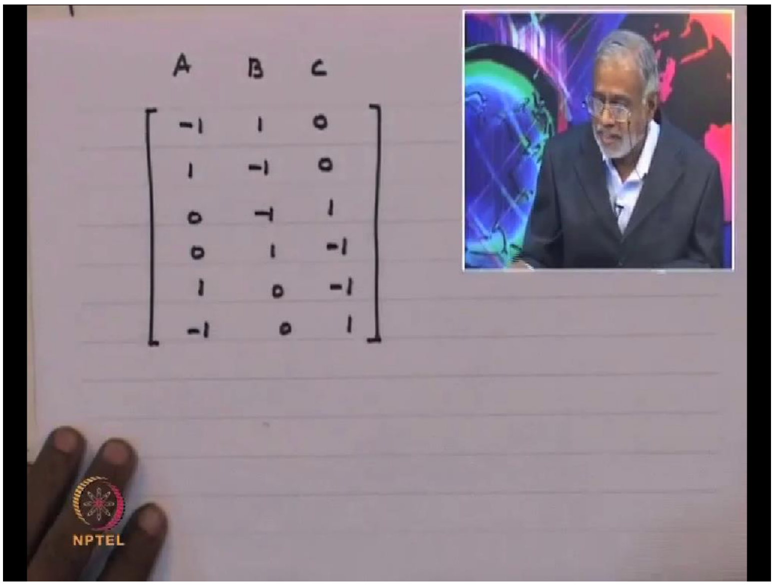

If you see, it will take much longer time, but the fact is that it is very obvious that the rank is still 2; it is not going to change the rank. So, the rank of this matrix; whether, it is single reaction or reverse reaction and so on, the rank is 2. Therefore, to be able to understand what happens to this reaction set in a process, you only have to take two of these three reactions. Any two, you can take and write a sticheometry. So, what I want to do now, is do the same thing in two or three different ways, just to illustrate how things play out.

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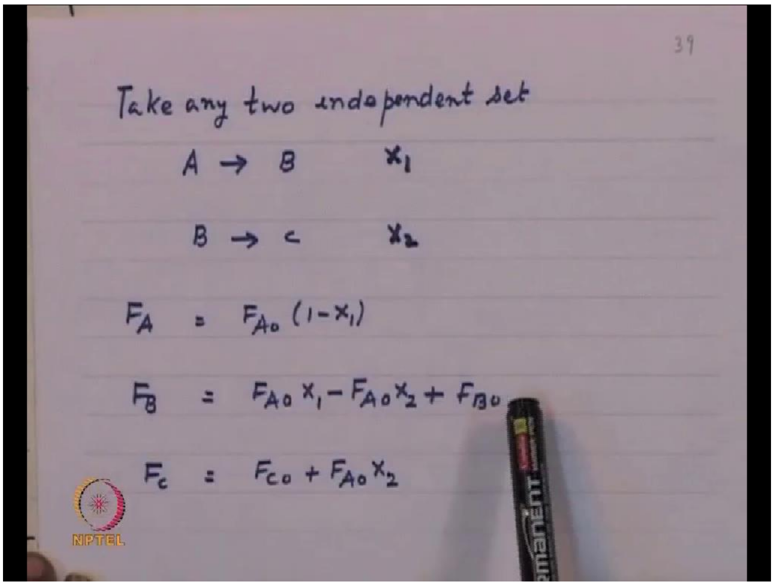

So, I have taken first independent set; A goes to B; B goes to C; this is our independent set; first example. So, what is F a? What is F b? What is F c? Assuming that x 1 is reacting here, I have written F a is F a 0 times 1 minus of x 1. If x 2 is reacting here, I have written the difference in F a 0 x 1 is formed; F a 0 x 2 is reacting and therefore, F b is so much. Similarly, F c; whatever is formed is due to this reaction. On other words, what we are saying is that if this is x 1, and this is x 2, then this is the sticheometry table, tells us how much is the material flowing at any point in the equipment. Now, all these reactions are instantaneous. Instantaneous means what; we can say that each of those rate processes are in equilibrium.

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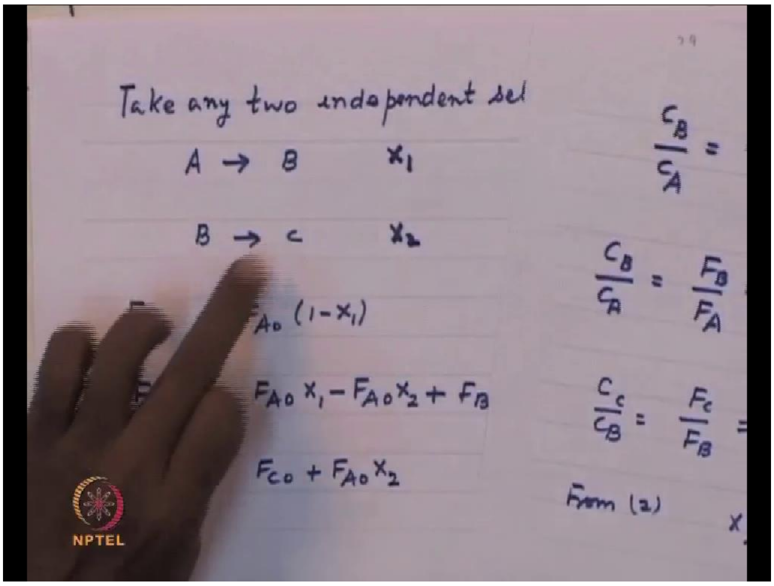

So, this kind of relationship should hold, which means what; A and B are in equilibrium; B and C are in equilibrium.

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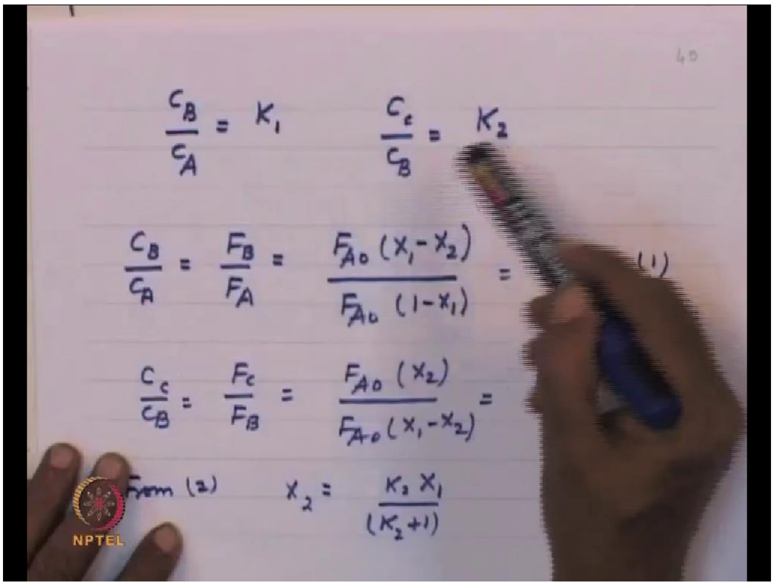

Therefore, C b by C a is k 1 and C c by C b is k 2 and therefore, we can calculate what is, I mean, I have just written down what is C c and what is C b, all that. We can just look at here. So, F b is F a 0 to x 1 minus x 2; F a is this; F c is this and F b is this. So, this states two equations in x 1 and x 2, involving k 1 and k 2. So, we can find here, x 2 from 2.

This equation, we can find x 2; we can see straight away; it is k 2, k 2 x 1, divided by 1 plus k 2, and you can take it forward from equation 1.

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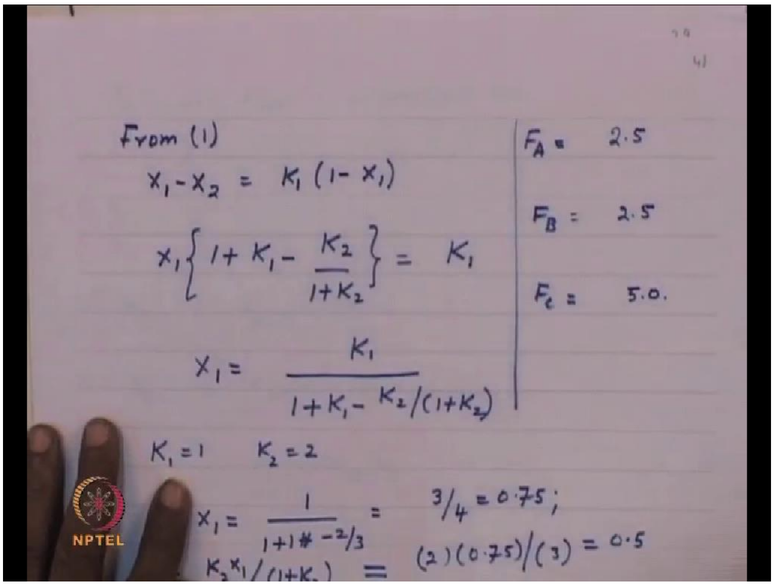

If we look at this equation, and then we can resolve this and say that x 1 is this; x 1 is given by this relationship; x 2, we have already shown.

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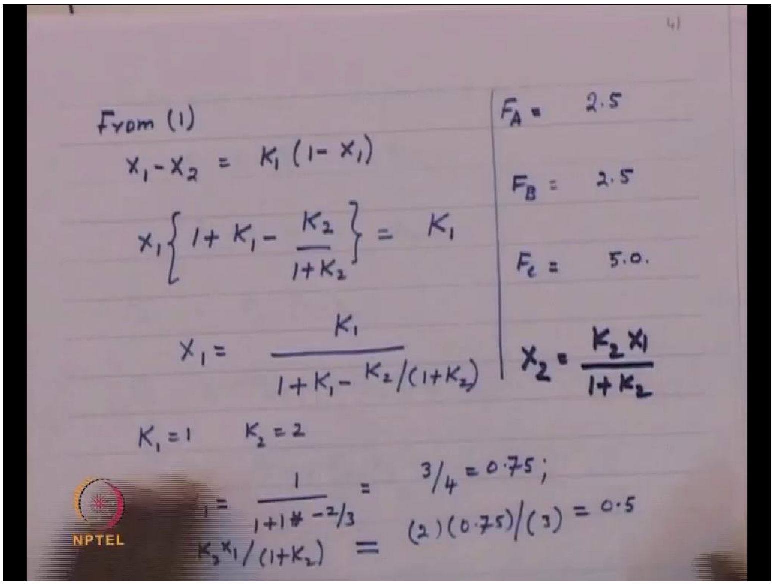

X 2 is equal to k 2 x 1, divided by 1 plus k 2. So, this comes from the equilibrium relationships. Since, k 1 is given as 1; k 2 is given as 2; you can find out x 1 and x 2. So, what have we done? Yes, there are six rate processes. Even then, we have taken only two reactions. We have taken arbitrarily, A going to B; B going to C, and then we set up this, and then we got the results. Once you know x 1 and x 2, you will find, calculate F a, F b and F c, correct. Now, we can do the same thing in a slightly different way; that means, what I am saying is that let us say, as an example.

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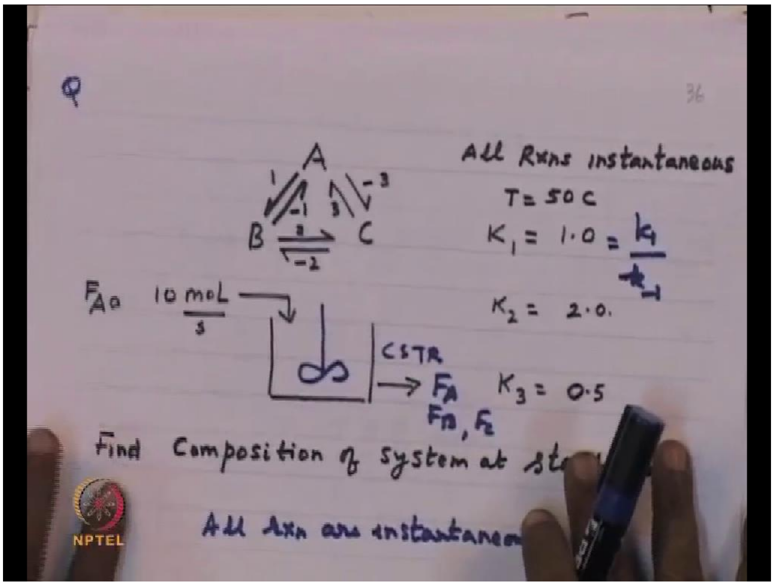

In this exercise, I said F a 0 is 10; that is why we set up all this where, F a 0 is the basis, correct. Now, suppose I say, no, it is F c; it is actually, material coming with F c is 10 moles per litre. F a and F b are 0; what changes? How do you formulate the same problem?

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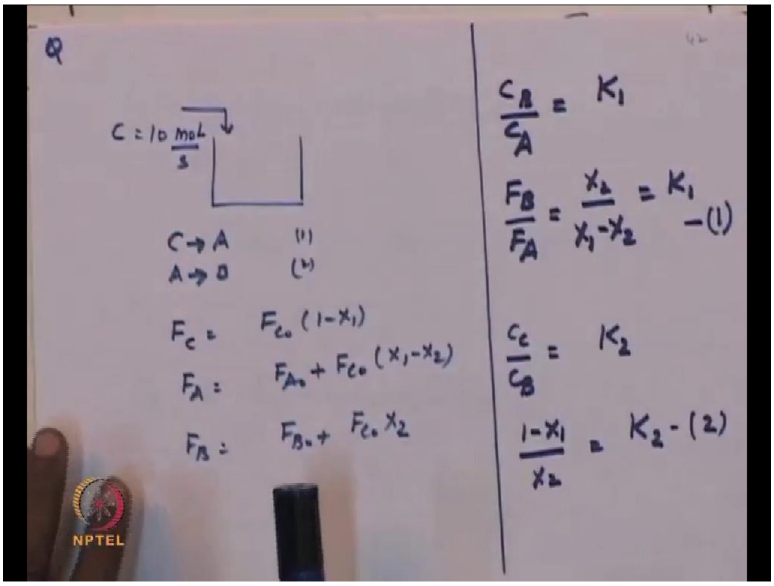

What I have done is let us say, C goes to A; A goes to B. So, the F c is 1 minus x 1; F a is x 1 minus of x 2; F B is F c 0 times of x 2; is the logic clear?

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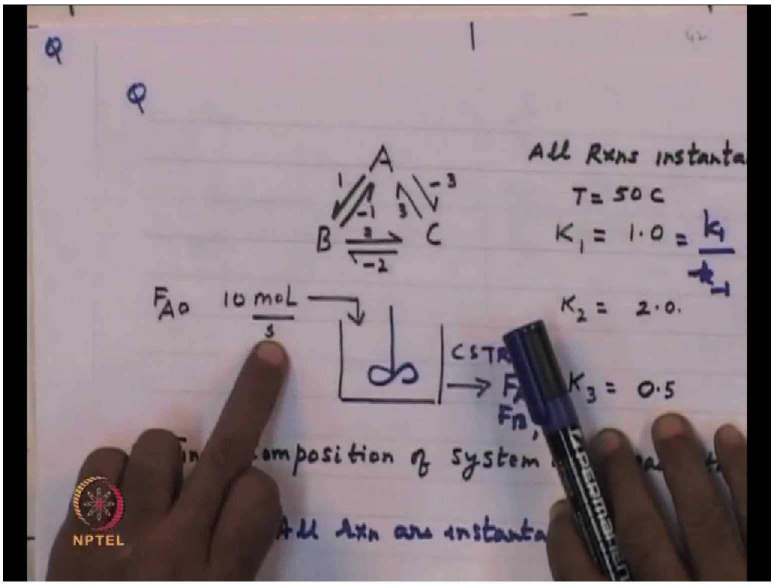

Instead of the previous case, where I said A is 10 mole per second.

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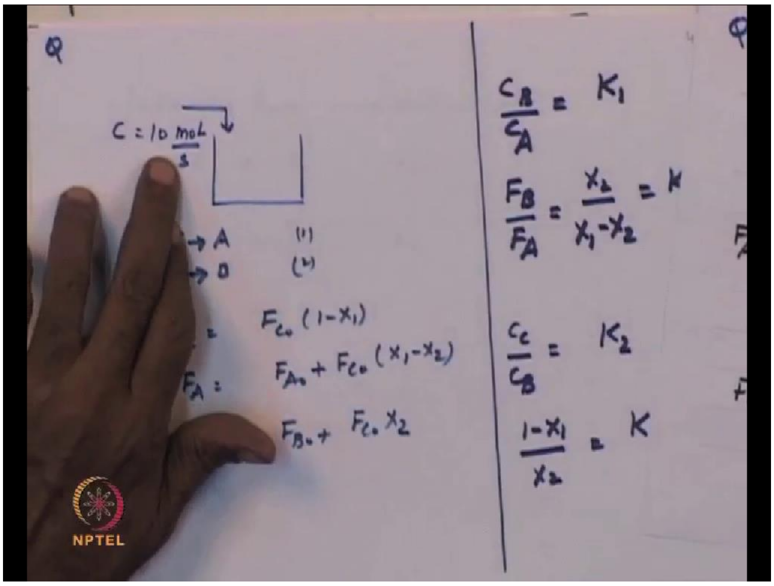

Now, I am saying same system, F c is 10 mole per second. So, sticheometry does not change, but we write the sticheometry in this form. How much is C; F c 0 multiplied by 1 minus x 1. Why it is 1 minus of x 1; I have taken this as x 1; I have taken this as x 2. So, you can write how much is A? A, this is formed here, and consumed here; therefore, I put x 1 minus x 2, and B is formed in reaction 2; therefore, plus x 2.

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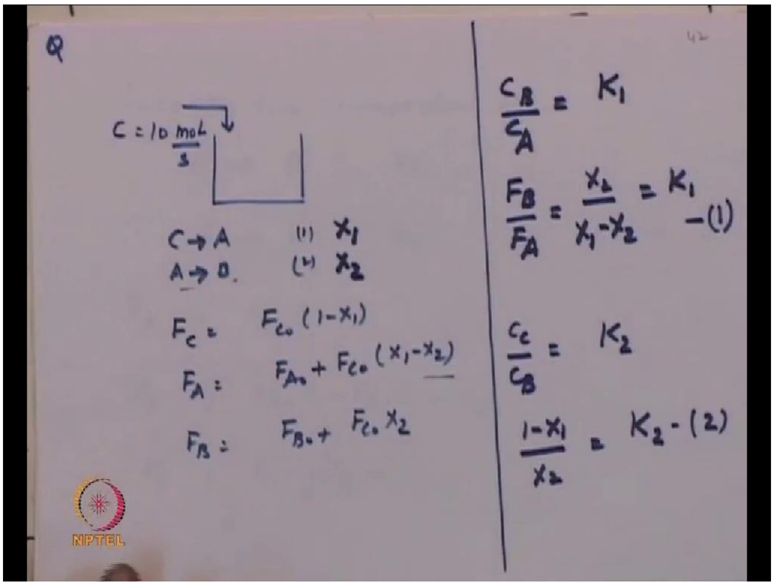

Once again, we can go through this and solve, but when you try to solve this, you find the way it plays out is not identical to what we have done, because now; I solve this here, just look at; just taken C b by C a is k 1, and then C c by C b is k 2. So, you have these two equations, x 2 by x 1 minus x 2, equal to k 1, and then 1 minus x 1 by x 2. It has come from here only; both. So, you have k 1 equal to x 2 by x 1 minus x 2 and k 2 equal to 1 minus x 1 by x 2. Two equations, we can solve.

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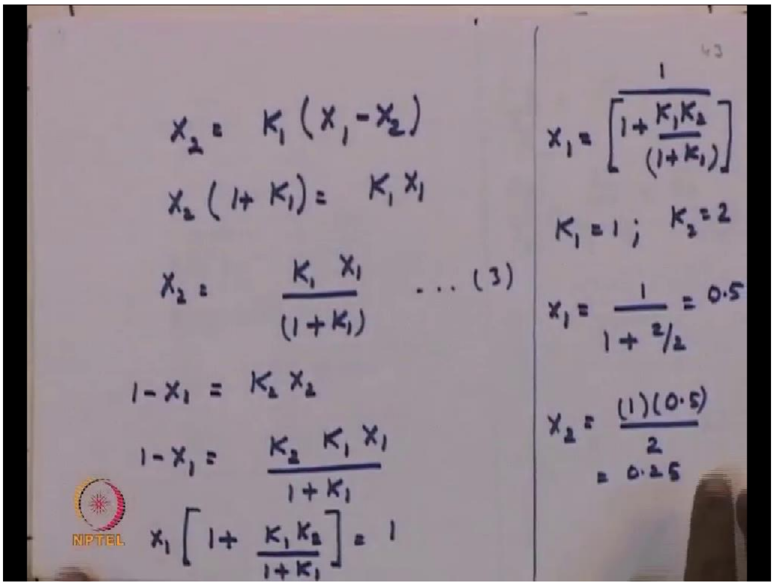

When you solve this, what you can get here is this; x 1 turns out to be this; x 2 turns out to be this. So, it is fairly elementary.

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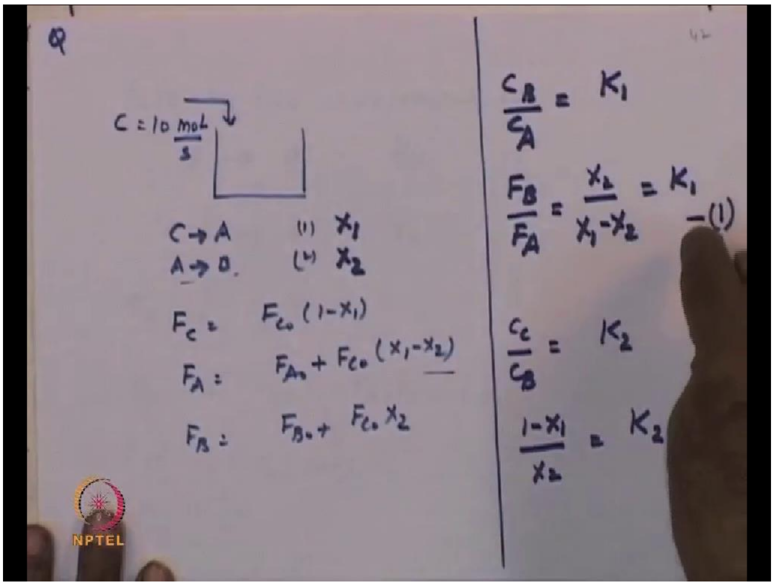

This is equation 1 and this is equation 2; x 2 and x 1, we can solve this which, I have done.

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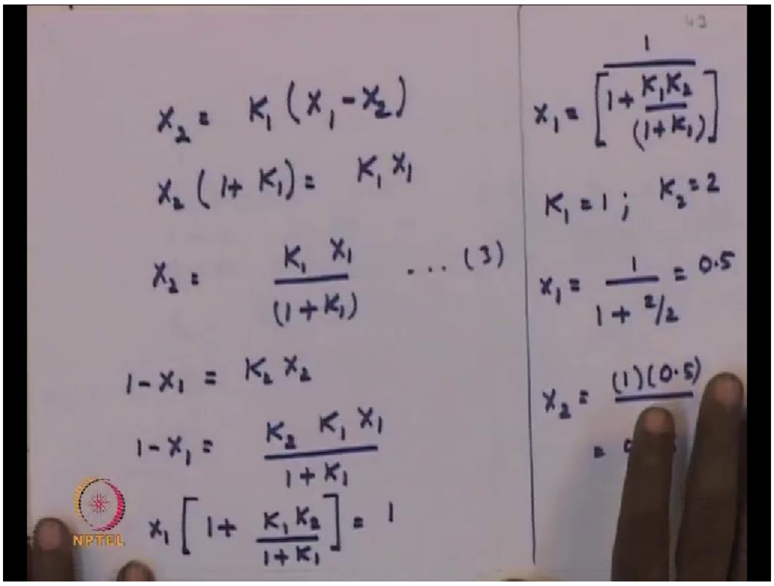

So, you got here, x 2 is this; x 1 is this. Once you know x 1 and x 2, your sticheometry is already set out. So, you can calculate.

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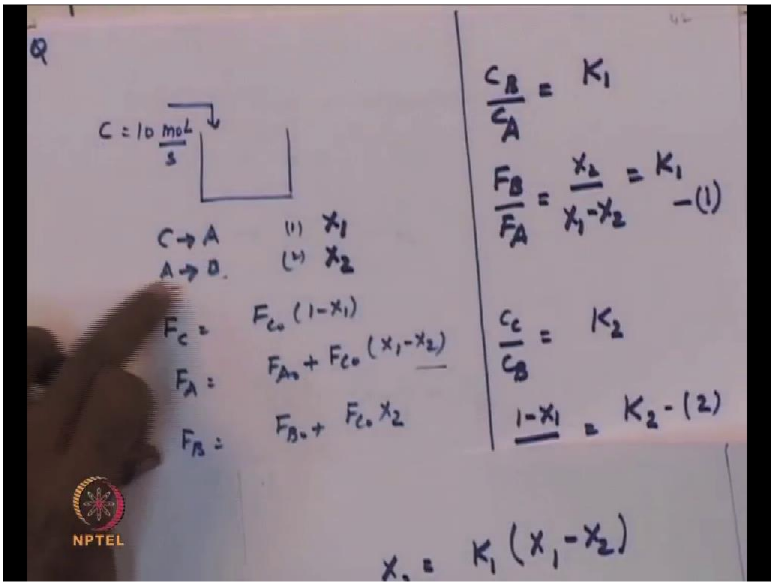

This is the sticheomeetry, is C going to A; A going to B. So, we can calculate what is F a, F b and f c; is this clear? Procedure is the same. In one case, F a 0 is coming in;

another case, F c 0 is coming in; that is the only difference. Now, when you do, when you substitute values of F a and F b and F c values of x 1 and x 2; what you get for F a, F b and F c is this; 2.5, 2.5 and 5 adds up to 10. So, it satisfies the material balance also. Now, what we have done in these two exercises is that by looking at the form of the chemical reactions, we have taken some things as our reference. First case, we took A as our reference. Second case, we took C as our reference. Suppose, you are dealing with a biological reaction where, thousands reactions are occurring; very difficult to even, identify which is the reference species we should take. It will not be easy to determine. So, you need something, which is able to handle thousands of reactions. How do you do this? So, let us do the same problem in a slightly different way. So, what is the problem you want to solve?

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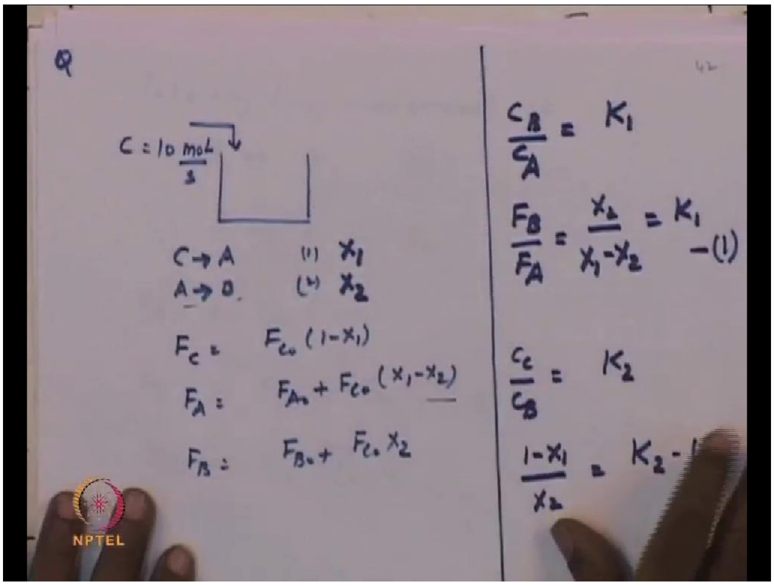

You want to solve for the case; I have just taken this example; C is coming in as 10 moles per second. I want to solve this problem. I want to find out what is the value for F a, F b and F c. We have already solved this problem. We know the answers, but you want to repeat this using the general approach that we have given in our class. What is our general approach?

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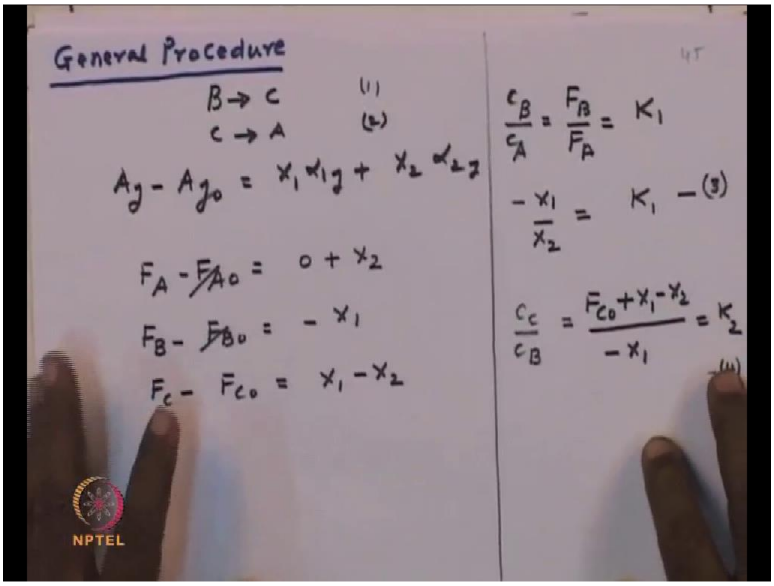

What we said was that if there are large number of reactions are occurring; let us say, a j minus of a j 0 is x 1 alpha 1 j plus, x 2 alpha 2 j upto, x r alpha r j, correct, where r is the number of independent reactions. So, x 1 is the extent of reaction in first independent reaction; x 2 is second independent reaction. What I have taken for this network; A going to B, going to C; let us for the moment, choose two reactions. I have just taken B going to C; C going to A as an example. You can choose any. So, there are two reactions. This B going to C; this x 1, the extent of reaction is x 1; C going to extent of reaction is x 2, correct. So, when you write a j minus of a j 0 is x 1 alpha 1 j plus, x 2 alpha 2 j. Now, I want to write the stoichiometry for component A, component B and component C.

Let us try to do that; that means, a j minus of a j 0 is F a minus of F a 0. What is x 1 alpha 1 j here? For component A, what is alpha 1 j? Alpha 1 j is 0. What is alpha 2 j? Plus 1. So, F a minus F a 0 equal to 0 plus x 2. Now, F b minus F b 0; F b in reaction 1, F b has a negative sign; minus 1 in reaction 1; B occurs in reaction 1; it is minus. So, I put minus x 1. X 2 does not occur in the second reaction. So, I should put 0. Now, go to the next one; F c; F c minus F c 0 equal to x 1 alpha 1 j; C is plus 1 x 1, and then x 2 alpha 2 j, C is minus 1. So, it becomes x 1 minus of x 2. What we have done now? We have taken a general case, B going to C; C going to A. You just selected two of the reactions that are occurring. What I am trying to say is that when you are dealing with large number of reactions, this is what you will do. You just select some reactions which, you think is an independent set, based on your matrix analysis. Having done that, we have written the sticheometry. Now, the problem specifies that the reactions are in equilibrium.

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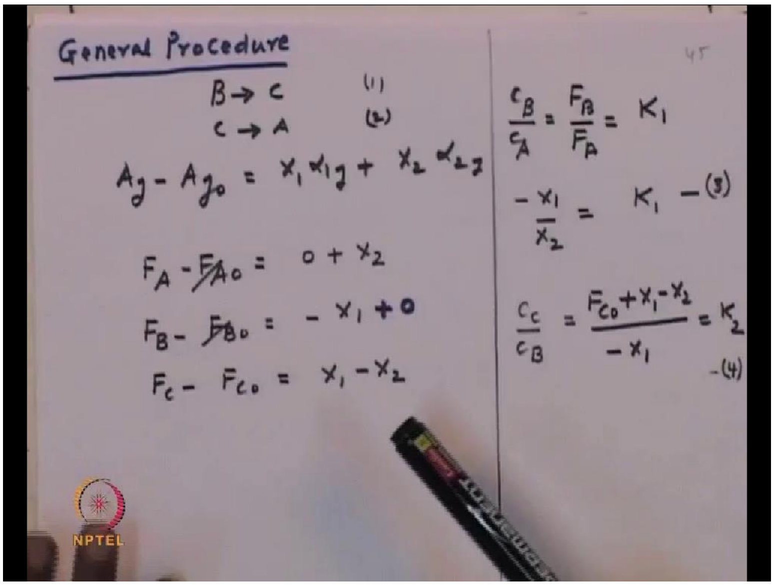

Therefore, C b by C a must be F b by F a is k 1.

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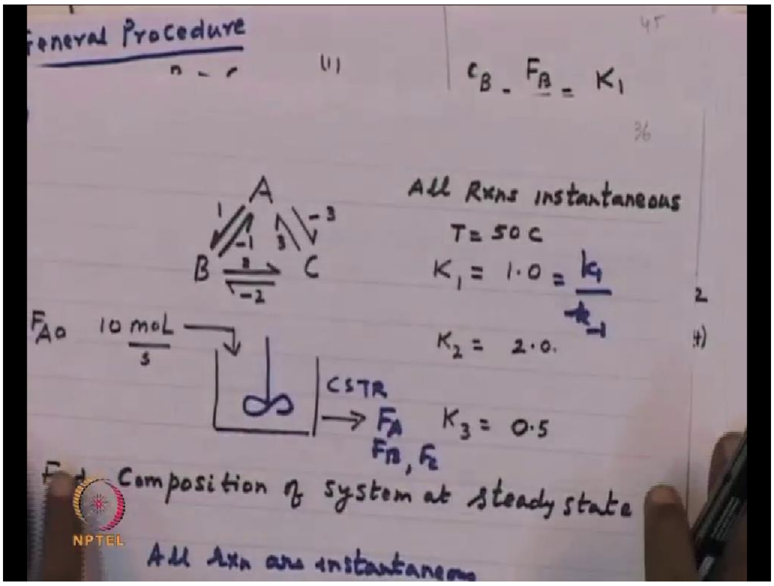

What have done is, please, your point is well taken. What is given to us is A to B is k 1; B to C is k 2; it is given. I can calculate the rest; I have not done that. So, what is given is that equilibrium constant A to B is k 1; that means, C b by C a is given as k 1 and B to C is given as k 2, which is C c by C b is given as k 2. That is why I did not make any change there, because that is what was given, anyway. So, this does not alter the result, anyway. So, what is given is C b by C a is k 1; C c by C b is k 2; it is given to us. Now, you have to write this in terms of our stoichiometry. What is our stoichiometry?

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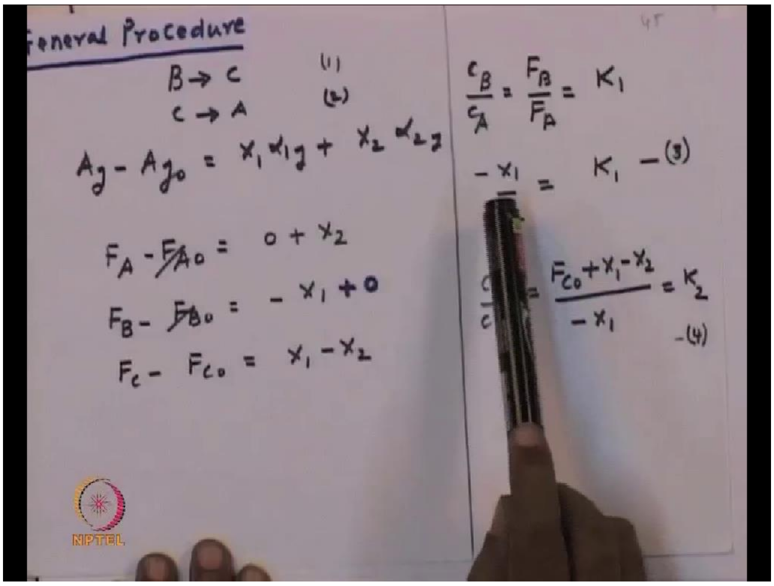

It says minus of x 1; F b by F a is minus of x 1 by x 2 is k 1; is it all right; minus of x 2 by x 1 is k 1, and then we have F c by; this is F c by F b, correct. So, F c is what? F c 0 plus, x 1 minus of x 2, and then divided by F b is minus of x 1. So, we have two equations; 3 and 4, which to solve for x 1 and x 2. Can you help me please? Please, solve for x 1 and x 2 for the case where, minus x 1 by x 2 is k 1, and then this is equal to k 2. We can solve for x 1 and x 2. Now, please solve and tell me the result. I will write the result. Just tell me whether, this is OK.

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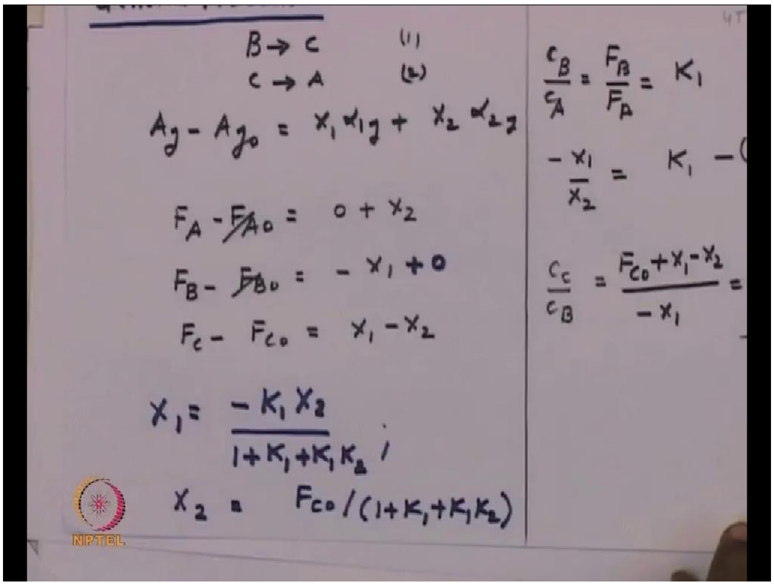

I will just write the result, and then we can check. Then, the other one also, you have to do. So, this is the result that I get; x 1 is minus of k 1, x 2; 1 plus k 1 plus, and x two is this; do you all get this? X 1 is also correct; x 2 involves F c, anyway. Do you all get this x 1 x 2? It is important, because it is something important to be said; that is why I am saying. Please remember, x 1 comes from k 1 x 2; this comes from here; minus, not x 2. So, this is the result I get; is this correct?

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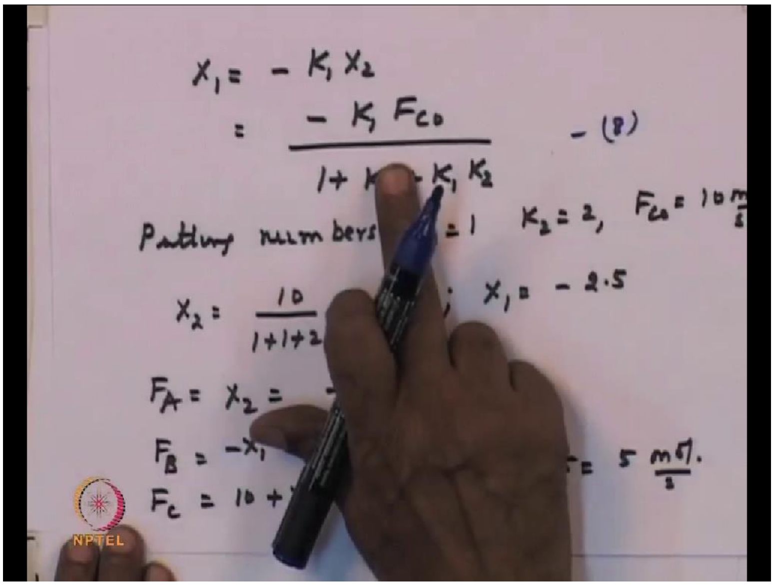

X 2 is what; this is what I get; is it correct? Now, you know x 1 and x 2, correct. X 1 is known; x 2 is known. So, this result is correct. So, please find out what is x 1; k 1 is given as 1; k 2 is given as 2. So, we can find out x 1 and x 2. What is x 1 and what is x 2? X 1 is; where are we; minus 2.5. X 2 is 2.5. So, what is F a b and c; F a, F b and F c?

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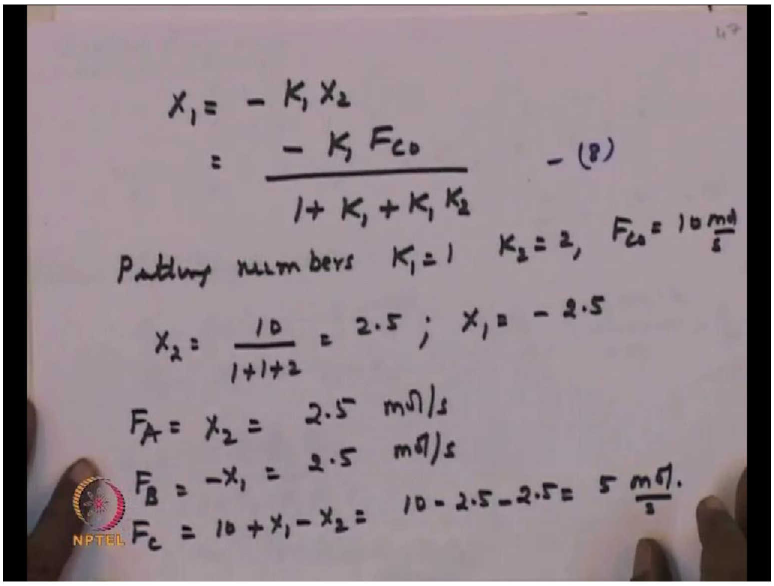

This is the result I get, F b, F c; F c is 5. We have solved the same problem a little earlier, if you recall, and then we got our results. See, I am just showing those results. See, we have F a; 2.5, F b; 2.5, F c; 5, correct. This is the same result that we have got last time, when we assumed. We did the same problem slightly, differently, but the results are the same.

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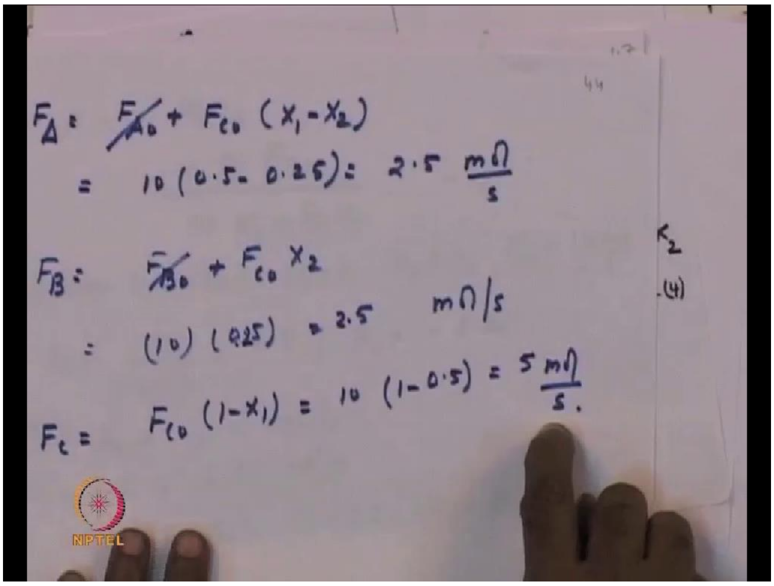

What I am trying to put across to you is that frequently, we find it convenient to choose a basis. It is generally, OK as long as this problem is small. When the problem is very large, number of reactions are very large, you will find that this technique of choosing a basis is not very convenient. Therefore, we have to go with this general procedure where, all these are not important. You just simply, select a set of r reactions, which are independent. How do you do this? We have done the matrix analysis. We can set, select the r independent reactions from our matrix analysis. Once you have done that, you can set up this stoichiometry, and then proceed with this.

Some of these excess may be negative; nothing to worry, because the choices are like that. Some of them may be negative; some of them may be positive; it does not matter. As finally, all the numbers you get would all be perfect; just like here, F a, F b and F c. Although, our one x was negative, but F a, F b, F c were consistent; there is no problem. So, what I have tried to do through this exercise is that the general procedure, that we are set out; may be a little inconvenient for small problems, because the basis is not obvious, but the advantages rely in very large systems, particularly, if we are dealing with biology where, the reactions are very many, is useful.

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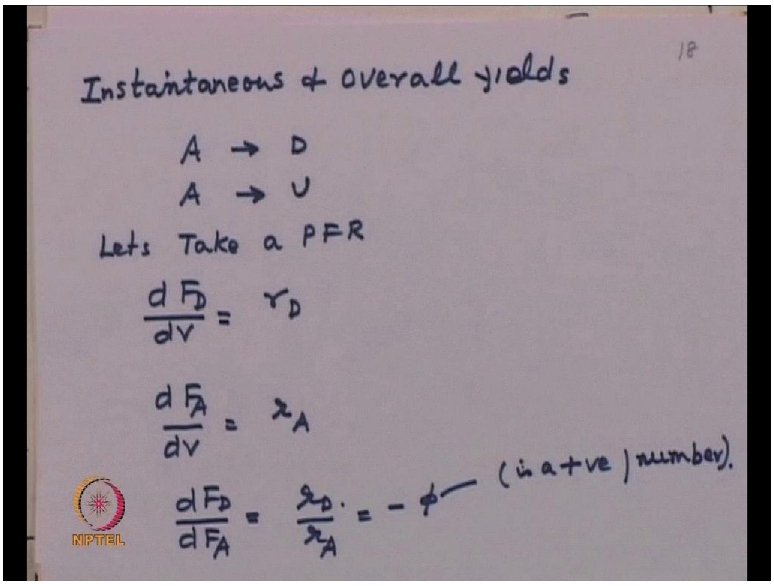

What is meant by instantaneous and overall yields? You know this is something that comes in extremely useful, when you are doing what is called as process development. You see frequently, what happens is that you set up a process, and then you are looking for a desired product and so many side reactions, do occur and therefore, there is an undesired reaction. When there is a desired product and there is an undesired product, then clearly, you need a way by which, you can maximize whatever, you have in your mind; whatever, you want to maximize. This whole procedure is trying to set out an experimental procedure by which, we can maximize our object; whatever, the object may be. So, to do this, what has been said is that A goes to desired product and A goes to undesired product. Therefore, when we conduct this reaction in a PFR where, therefore, we can write d F d by d v is r d. Similarly, d F a by d v is r a; that means, rate at which, F d goes to r d and F a goes r a. So, this ratio gives us what is called r d by r a; that means, rate of formation of desired product to the rate of consumption of the raw material is in the ratio of reaction rate r d and r a. On other words, the advantage of this way of looking at whole problem is that the right hand side, r d to r a, is a state function. The right hand side is a state function. Therefore, this can be determined in various ways, because this is a state function and therefore, it is denoted as minus of phi to indicate that r d and r a have opposite signs. This is consumed, and this is formed. Just to keep to positive, we have this phi or minus phi; phi is a positive number; phi has a meaning of instantaneous yield, because it is occurring at a ratio of two reaction rates. That is why it has a meaning of instantaneous yield. We can integrate this and represent it like this.

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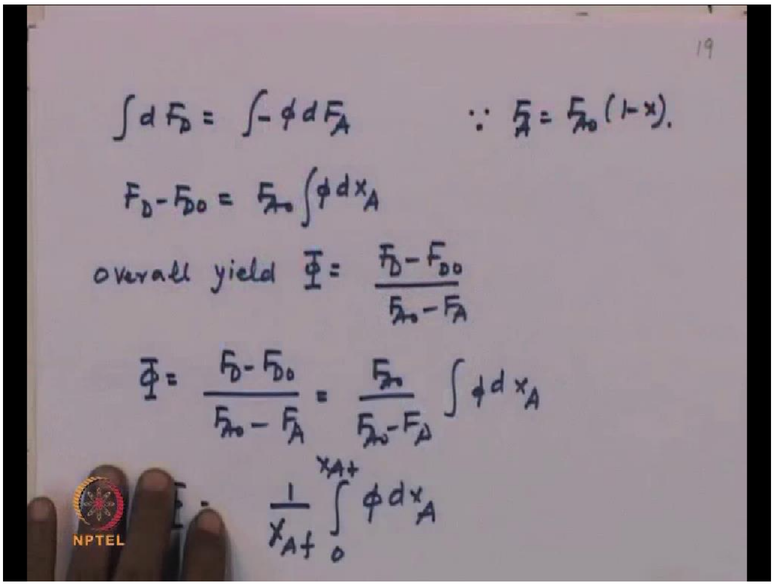

What I am doing now is simply, integrate; multiply this side, d F d, multiply phi by F a and integrate both sides. When we do that, what we get here is d F d, which is F d minus F d 0. When we integrate this d F a, because of this relationship F a is F a 0, 1 minus of x; the right hand side becomes F a 0 of integral phi d x a where, phi is the instantaneous yield. Frequently, our interest is what is the overall yield. What is overall yield by definition? By definition, is how much is the product formed, divided by how much is the raw material consumed; That is how we look at overall yield, correct. So, product formed to the raw material consumed. So, overall yield, if I call it as capital phi; it is raw material formed, sorry, product formed, divided by raw material consumed. So, that can we represented as this F d minus F d 0. What is this term? It is coming from here. So, it is F a 0 times phi d x a, and this term is F a 0, which is given as x a f. On other words, what we are saying is that the overall yield that you will get from a process is an integral of phi d x a where, phi is a state function, and phi d x a integral 0 to x a, divided by the overall yield. That gives you the overall yield. This representation, we will see shortly; it has several advantages. So, what we are saying here? Overall yield in a batch in a plug flow kind of device is integral of phi d x a, divided by x a f. Now, we can do the same experiment in a CSTR.

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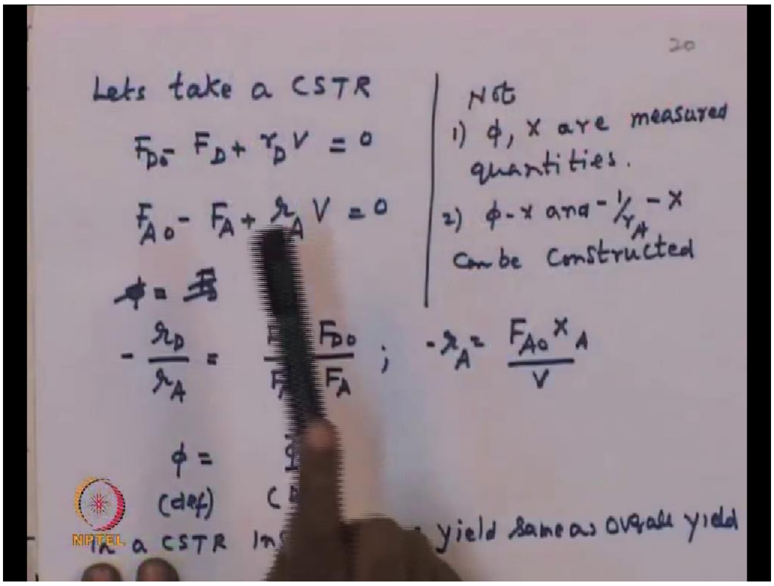

So, you have input output generation, equal to 0; input output generation, equal to 0. So, we can take these two ratios r d by r a, equal to F d 0; is this correctly written? Please check, have I written it correctly? F d minus F d 0 equal to minus of r d; F a 0 minus F a equal to minus of r a; is it correctly written? Yes, is it fine with all of us? Now, what meaning can you attach to this; r d by r a? We say it is instantaneous yield. What meaning can we attach to the right hand side? Overall yield. What are we saying? In a stirred tank, instantaneous yield is equal to overall yield. In a stirred tank, single stirred tank, instantaneous yield is same as overall yield.

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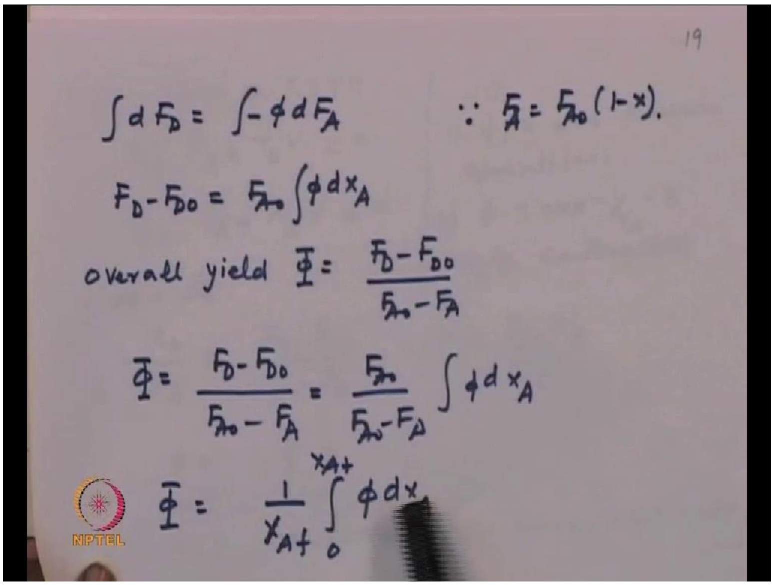

While, in a PFR, instantaneous yield; overall yield comes as an integral of phi d x a, divided by x a f. On other words, overall yield shows you an average in the equipment in a PFR. While here, it shows up directly, is something that we all know. Now, let us look at the system carefully. What is phi? Phi is a ratio of r d to r a, correct; it is instantaneous yield. Suppose, I want to measure; what will I do? I run a CSTR experiment. I can run a CSTR experiment, so that, I measure r d to r a simply, by this ratio, because I can measure F d and F a and therefore, I know the right hand side. Therefore, I can make a plot of phi versus x. So, if i want phi versus x data, what would I do? I would run a CSTR experiment; is this clear to all of us? If I want to get a data on phi to x, what will I do? Because CSTR directly, gives me phi and this gives x also and phi. So, CSTR gives you good data on selective instantaneous yield versus conversion. So, you are able to plot from your CSTR data, x versus phi, correct; is this clear?

Now, what is this data; minus of 1 by r a versus x? Can we get that data from that same experiment? On same experiments, there are two exceeds. You are doing a experiment so you are able to measure f a 0; you are able to measure f a. You are able to measure r a. Therefore, your 1 by r a versus x is also known to you, because it also comes from the experiment. So, a CSTR experiment gives you two valuable results. One result is that it gives you minus of 1 by r a versus x; second result, it gives you that how phi is related to x; is that clear? So, both the data comes out of your CSTR experiment.

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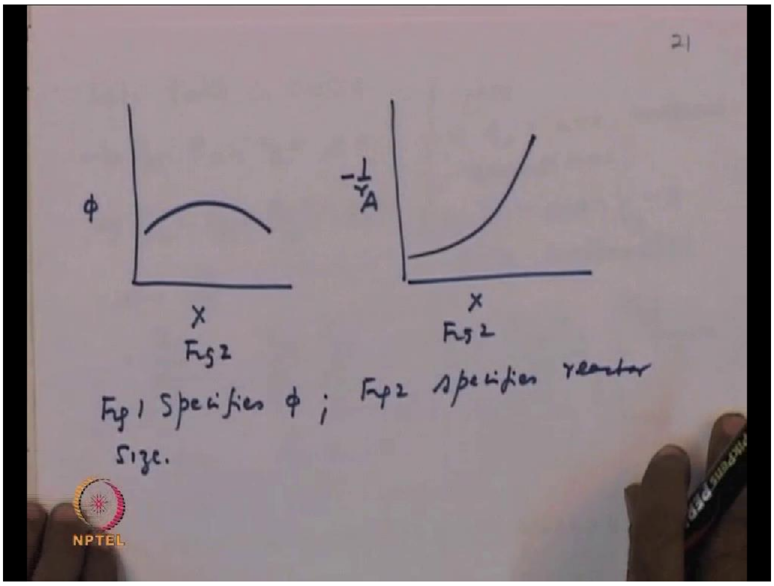

On other words, what we are saying now, is that through your CSTR experiment, you can generate data on the system time to investigate, without any knowledge of the chemical kinetics, because chemical kinetics in many cases, are so complicated that the effort involved in getting that function is not easy, but this may not be so difficult, because this is an easier experiment to do. So, you can generate phi versus x data and minus of 1 by r a versus x data. Now, you have all the data in your hand. Various kinds of questions, associated with reactor design and reactor optimization, etc can all be answered now, because you have the data, and you have, of course, experimental points. Therefore, most of your numbers come out by graphical integration kind of answers, but in any case, it is supported by experiments.

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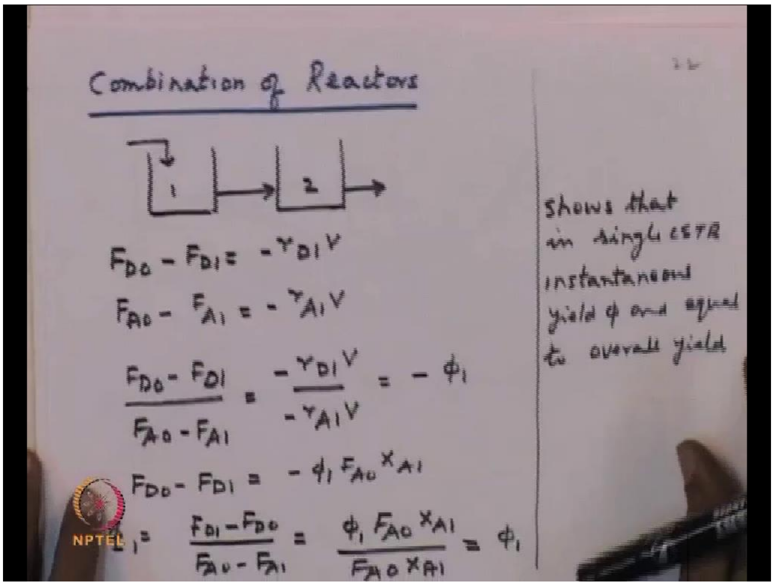

So, with this, suppose now, I ask you; suppose, we have a combination of reactors, which means what? You have two stirred tanks put together. Let us see what is the overall yield that we will get when, two stirred tanks are together. What we are trying to say is that you already have this data, phi versus x. These data are already with us. Now, we want to see how we can make use of this kind of data by our fundamental understanding that we have about stirred tanks. Now, what I have got here? I have written for tank 1; input output generation equal to accumulation; is this OK for desired product? Input output plus, r d; I have written on the right hand side. Similarly, there is component A; input output equal to minus of r a 1 v. So, we can take a ratio and you get result which, you already know. What is that? F d 0 minus F d is given by this result, showing that overall yield is same as instantaneous yield; something that we already know. I am stating it once again. For tank 1, our result phi 1 is equal to small phi 1, showing that overall yield at tank 1 is same as instantaneous yield; that we already said. We are just stating it once again.

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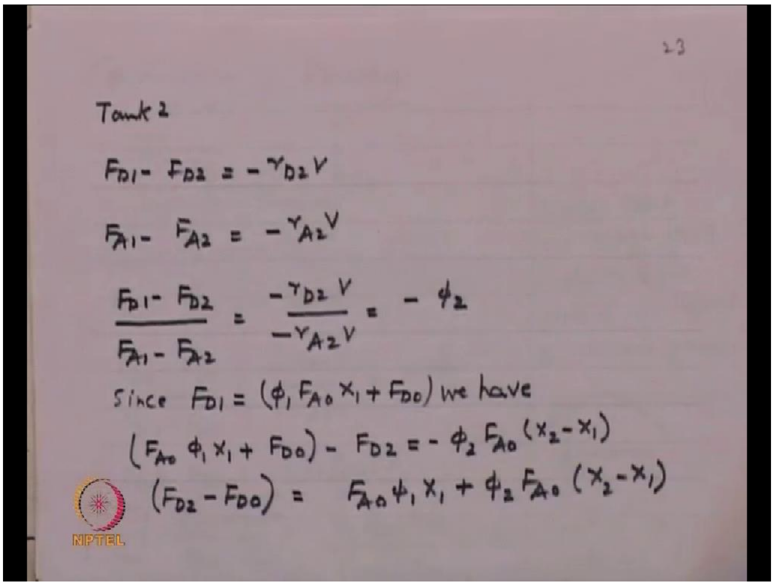

Suppose, let us go to tank 2. What does tank 2 tell us? Input output plus, generation; I have taken it to the other side; input output (()); this for component D; this is for component A. Ratio, if we take, what does it tell us? It tells us that F d 1, F d 2, F a 1, F a 2, r d 2, r a 2; what is the meaning of r d 2 by r a 2, because it is a stirred tank; it operates at the exit condition; therefore r d 2 by r a 2 is phi 2. Therefore, F d 1; what have done; F d 1 replaced it from here; F d 1, we have got already here; F d 1 comes from here. So, I just replaced it from the previous page. So, what you get here is that is F d 1 in terms of phi 1 x 1; F d zero stays; F d 2 equal to phi 2 x 2 F a 0 x 2 minus of x 1; is this clear to all of us? How this phi 2 F a 0 x 2 minus of x 1 comes? What it means is that now, F d 2 minus of F d 0, now, comes in terms of phi 1 x 1, phi 2 times of x 2 minus of x 1; you understand. So, what we have now said is that the product that we are making in the second tank; F d 2 is the product that comes out of the second tank, that depends on F a 0 phi 1 x 1 phi 2 F a 0 x 2 minus of x 1.

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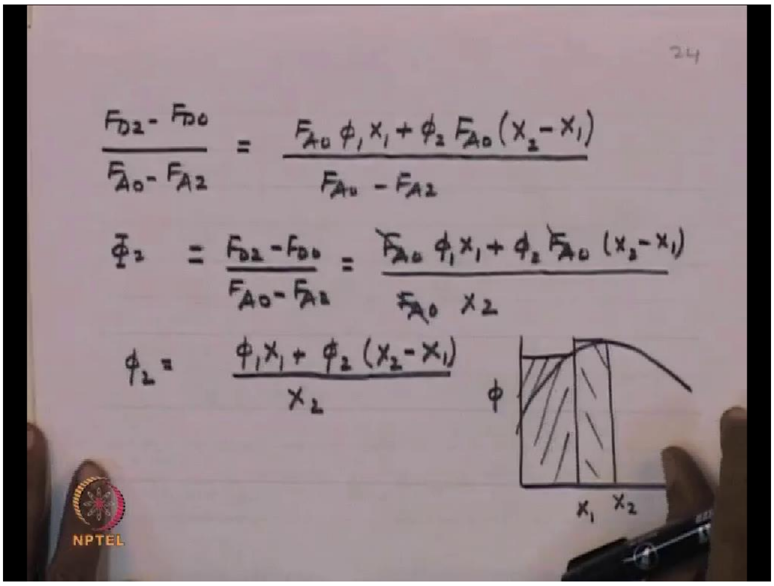

So, it is now expressed in a very convenient form, which is what overall yield equal to phi 1 x 1 plus, phi 2 times of x 2 minus of x 1; that means, if you have this function here overall; this is the data that we got from our experiment, correct. So, in the first, the overall yield that you get in two tank sequence, is what; phi 1 x 1; that is this triangle; this rectangle plus, phi 2 times; phi 2 is this point; phi 2 times x 2 minus of x 1; this rectangle; you understand. You see, this is a very nice procedure, which is developed by Professor Denby in the 1940's. What is being said is that if you generate this curve, phi versus x, then you can use the same procedure that we have used for staging and multi reactor, I mean, size of the equipment; that we have done for a long time. The same procedure applies here also; that means, if we want to find out the overall yield of two tank sequence; first tank gives you this area; second tank gives you this area; is that clear? So, same procedures apply; this is what, is the interesting point of this procedure that has been set out; is it clear? This is for a two tank sequence. Now, let us look at one more example. What is this example?

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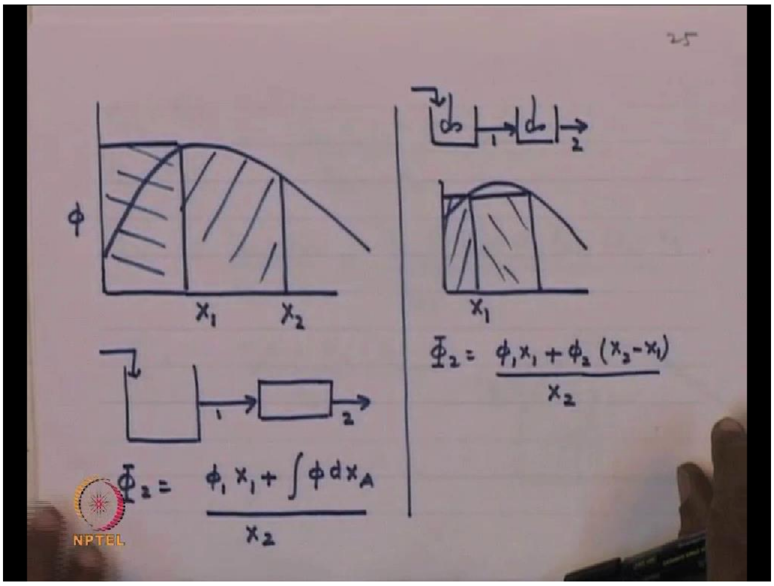

You have a CSTR followed by a PFR. What is the overall yield? Now, based on whatever procedure we have set up, straight away, you should tell me the overall yield will be, the first will be this area; second will be this area; that means, phi 1 x 1 plus, integral phi d x a by x 2. Same procedure, what we are said earlier. Here, we had a two tank sequence.

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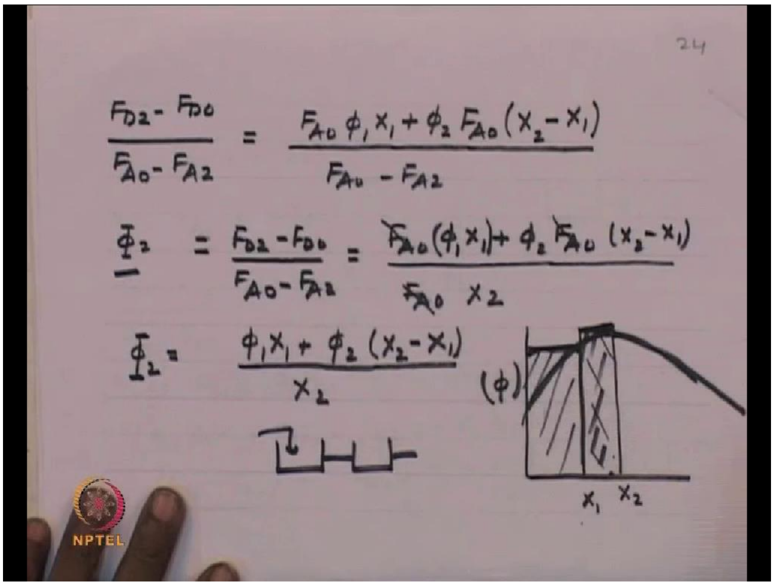

This is a two tank sequence. So, we said that it will be this rectangle and this rectangle; that means, second rectangle is constructed on this; first rectangle is constructed on this point, but if we have a CSTR followed by PFR, it is what; CSTR is phi 1 x 1.

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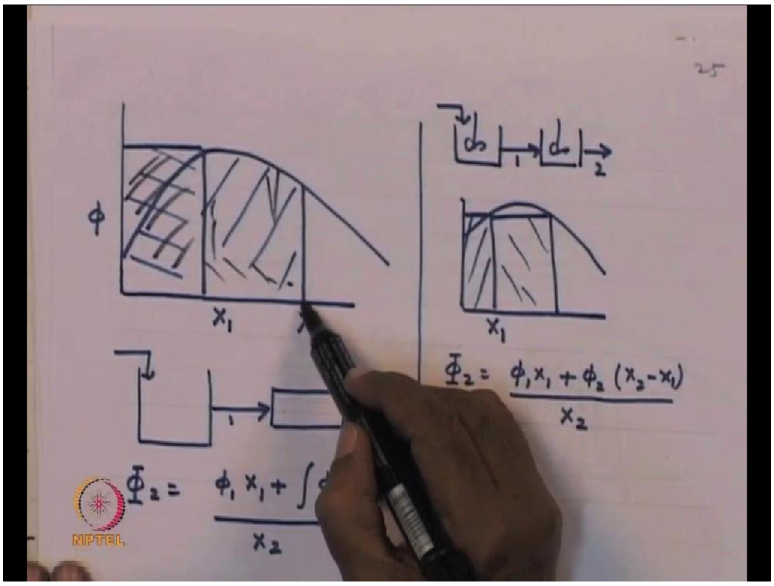

This rectangle, you can see, this rectangle, and then second one is integral; this integral, the integral of this area here, phi d x a, divided by x 2; x 2 is the final conversion. This is exactly, what we have learned in the previous, I mean, reactor design approaches. Now, if I ask you what is the overall yield for the case of this; you will simplify, say this is the answer. So, various combinations for which, we want overall yield; we can straight away get, because we know this data. This is what then, we pointed out that when we have most of these results came out when they were trying to develop explosives during the war where, kinetics, etc are very difficult to do; number 1. And the urgency, it may not have been worthwhile. So, that what you wanted was a design, which would actually, produce the product of your interest. So, in most cases, you will find that kinetic data comes after a very long time, but processed data that is required for design; this is sufficient for you to give the information that is required.

With this background, I want to quickly look at this exercise. We have an exercise here where, this is also; I have taken from Denby only. What it says is the following. Let me just read out what is the problem statement.

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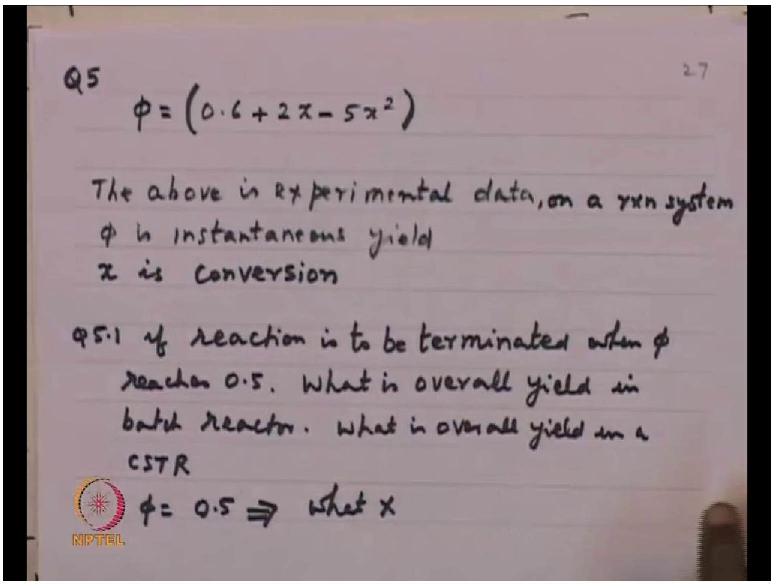

Problem statement is that experimental data on a reaction system, has been found to look like this where, the instantaneous yield is related to conversion by this functionality. Now, how does it come? We have said just now; it comes out of an experiment. CSTR experiments are relatively, easy to do. Even, if it is an explosive reaction, it is quiet easy to control temperature and make measurements. This is the great advantage of CSTR. You can measure even, very difficult reactions; you can manage to measure, because you are able to maintain temperature, quiet well, through an appropriate cooling. So, phi versus x data is given to you. Now, what is asked is if this reaction is to be terminated when phi is 0.5; that means, this is when phi becomes 0.5, we want to terminate this reaction. Why do you want to do this, because beyond that, it does not give you any benefits in terms of the product of your interest. So, what is the overall yield in a batch reactor? Is this question clear? If the reaction is to be terminated when phi instantaneous yield; phi is 0.5; what is the overall yield to be expected in a batch reactor? Is the question clear to all of us? What is the overall yield to be expected in a batch reactor? We said that just now.

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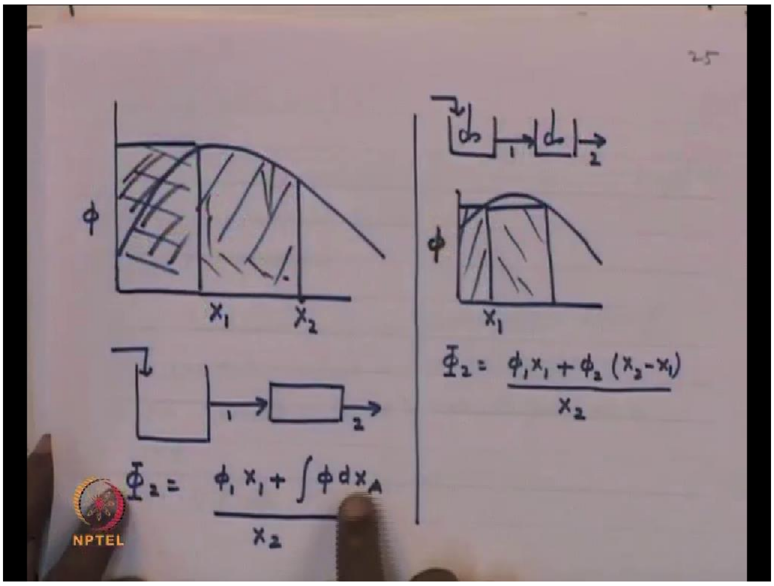

If you have a PFR, our overall yield is integral phi d x a, divided by final conversion. If it is a batch reactor also, it means the same thing; phi d x a, divided by x a, final conversion. So, the overall yield in a batch reactor is simply, integral phi d x a, divided by final conversion; is this all right what we are saying?

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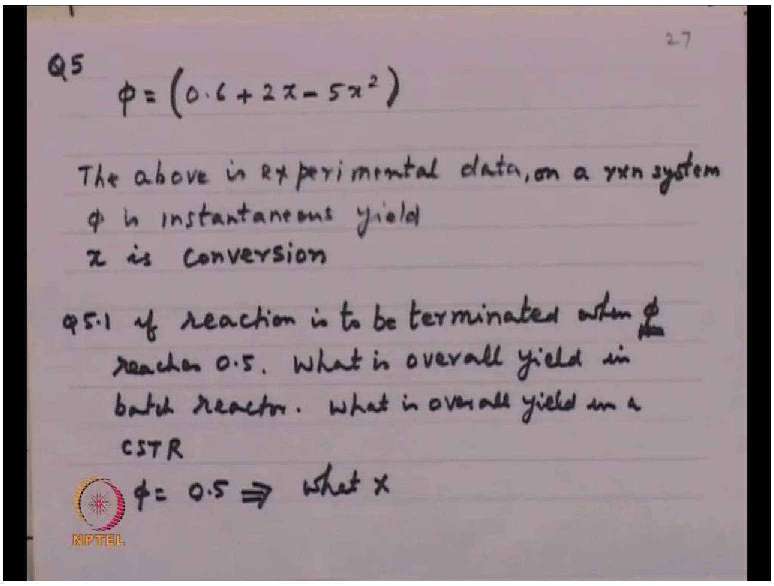

This function, that is given to you; it says what is the overall yield in the batch reactor. How would you approach this? Phi is given as 0.5. What is the expression for overall yield? We will say it is integral phi d x a, divided by x f, correct. So, how do you do this?

Student: (( )).

Prof: What will you get? What is the value of x?

Student: point (( )).

Prof: How do you find out?

We put phi equal to 0.5 in this; that tells you we have to stop at x equal to point, whatever that number is, 0.45. So, once you put x equal to 0.45; that tells you that phi becomes 0.5. You know the value of x. So, how do you find overall yield? We will find overall yield by our same expression that we have derived.

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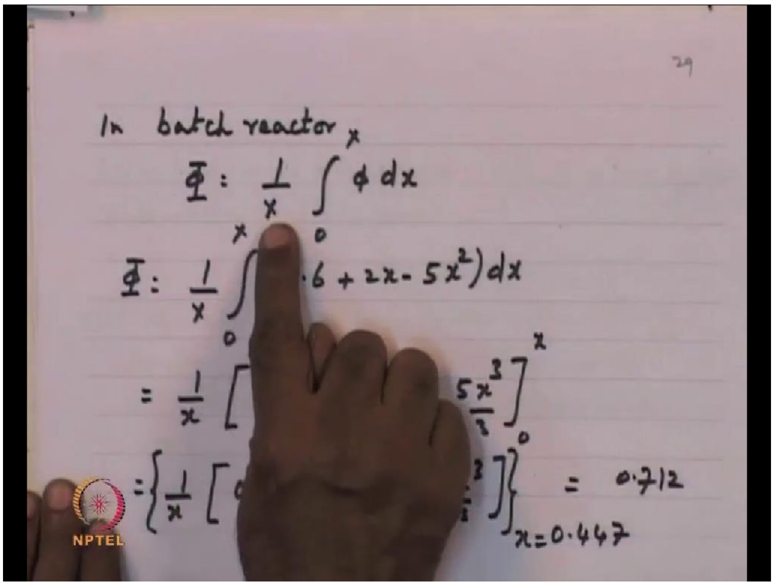

Overall yield is 1 by x, 0 to x, phi x d x; is this all right what we are saying? This comes from our understanding that phi d x integral 0 to the final value, divided by final conversion is the overall yield for a PFR or for a batch reactor; is this all right? Is this result correct, what I have got; 0.71; can you please tell me? Let us go to the next. Suppose we want to do the same thing now.

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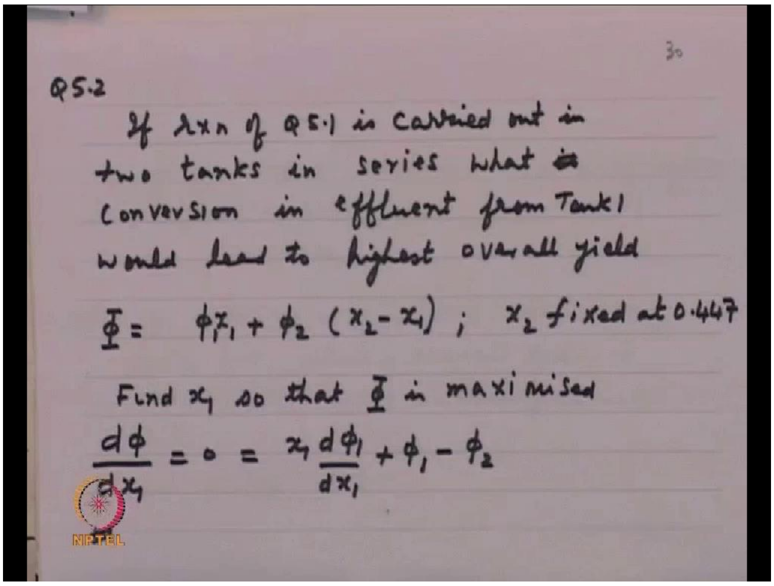

Second exercise is if this reaction is carried out in a two tank in series; there are two tanks in series; 1 and 2 series, what conversion in the effluent form tank 1 would lead to highest overall yield? What are we saying? Let us just recognize this.

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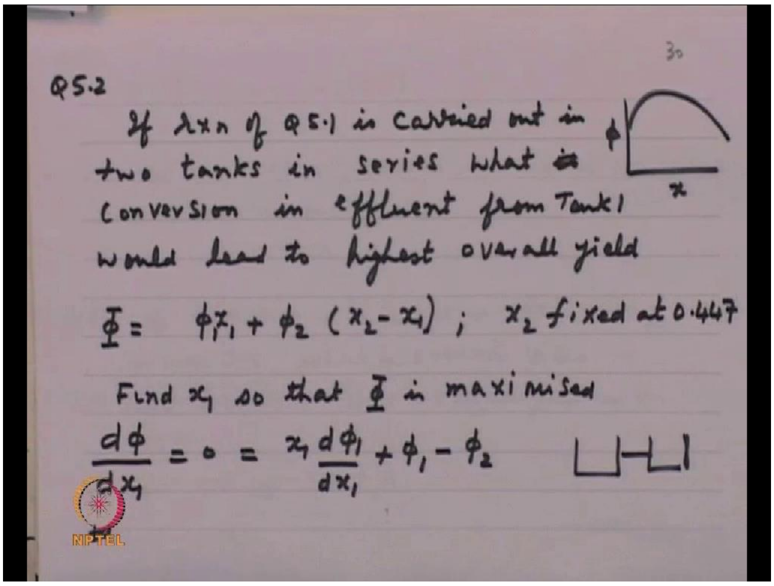

We have, this is our phi versus x curve; it says, it is a two tank sequence. You want to terminate this somewhere in between, so that, what conversion in the effluent from tank 1 would lead to highest overall yield? What would be our strategy? See basically, overall yield is determined by the area. Tell me, what choice of the intermediate point will give us the highest area. What choice of x 1 would give us the highest area? Let us try to answer this now.

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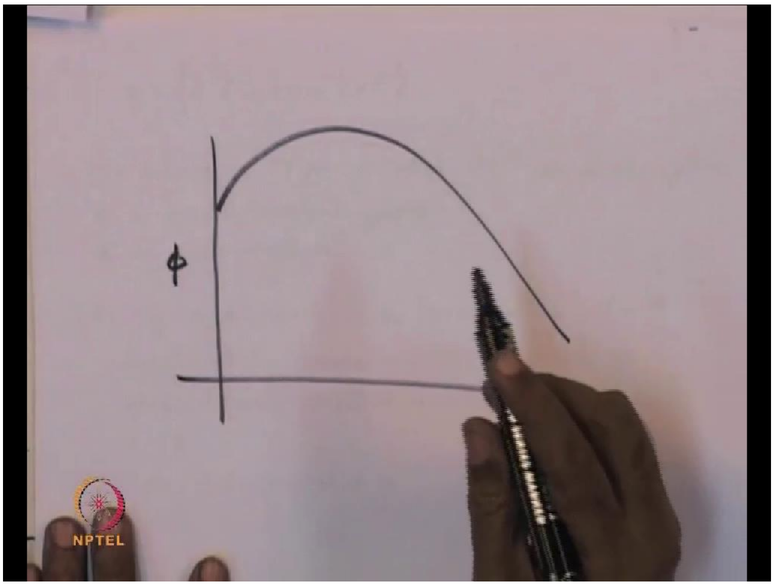

This is our function. So, this is how the curve looks like. What choice; you want to make a choice somewhere here, so that, the area; the overall yield is simply, an area, correct, but since, it is a stirred tank, does it say stirred tank? It says two tanks; both are stirred tanks, correct. What shall we do? You want to choose x 1. What I have done here is that we do not know what is that.

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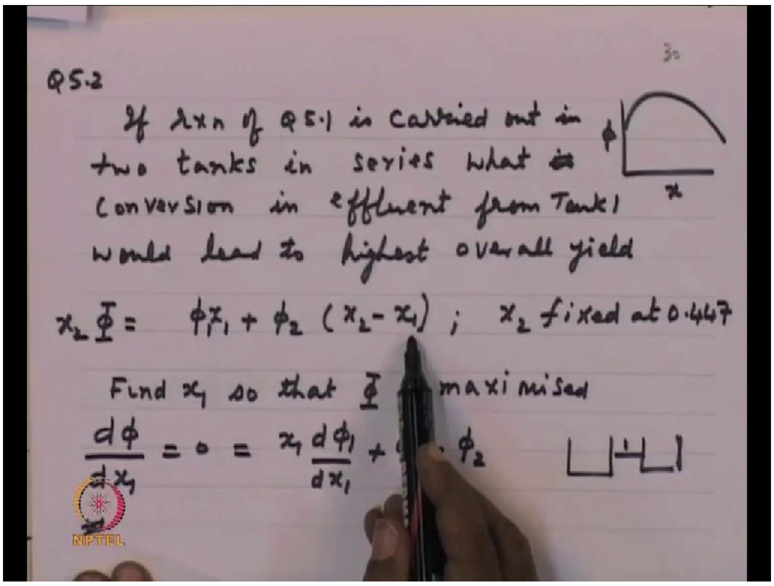

So, what I say, all right; we know that phi is given by; I should write x 2 here; x 2, I forgot to write; phi x 2 equal to phi 1 x 1 plus, phi 2 times of x 2 minus of x 1; this is the statement of the overall yield. So, we want to maximize; what is says is that we want to have choice of x 1, so that, the left hand side is maximized; x 2 is fixed. Suppose, we differentiate d by, if this overall by x 1 which, we do not know what is x 1 and said it is equal to 0. Then, we can find out the value of x 1 at which, this goes to maxima; is this clear what we are saying? So, x 2 is a constant; therefore, d phi by d x 1, this is the right hand side; d phi d x 1. Actually, x 2 can stay here; that does not create harm. Let us differentiate the right hand side with respect to x 1. How many terms you get? So, x 1 d phi 1 by d x 1; second term is x 1, and then when you differentiate this, you get minus phi 2. So, you have set it equal to 0. What is d phi d x 1? x function, phi function, is given here; phi function is given.

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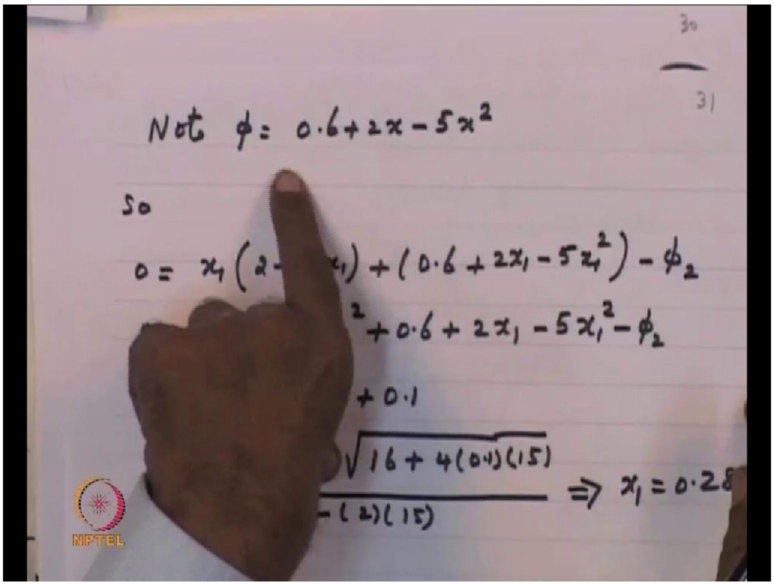

So, you know d phi d x 1, correct; is that clear? So, d phi d x 1 is known; therefore, you should be able to tell me now. Please tell me; please tell me the result. I get a value of 0.286. Please tell me whether, this is correct. I have done this; d phi d x 1 is equal to 0, which is equal to x 1 d phi 1 d x 1 plus, phi 1 minus phi 2. I put in the value for d phi 1 d x 1; all the numbers, etc; I have done this here. This is the result I get. Please tell me whether, it is correct. Is this result correct? Please, this differentiation is all that you have to do. See, what I have done; yes or no?

Student: Yes.

Prof: This differentiation is all right?

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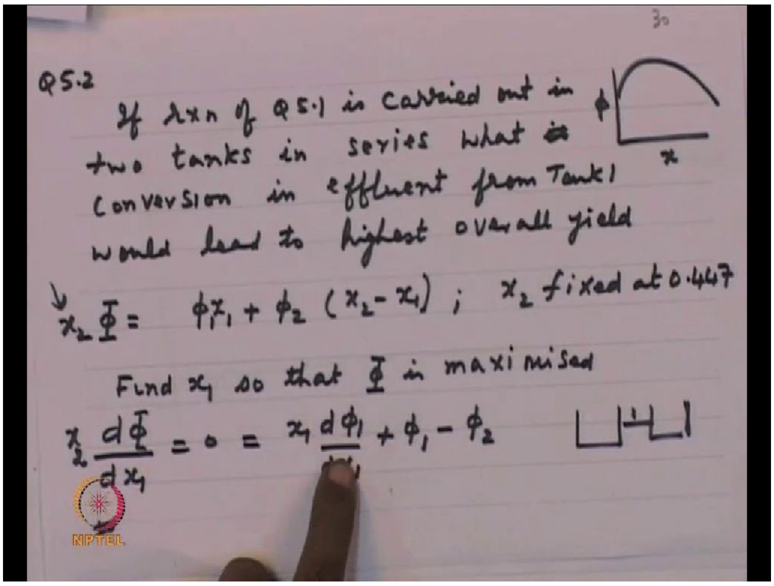

See, this comes from here; x 1 d phi d x 1; that function is known.

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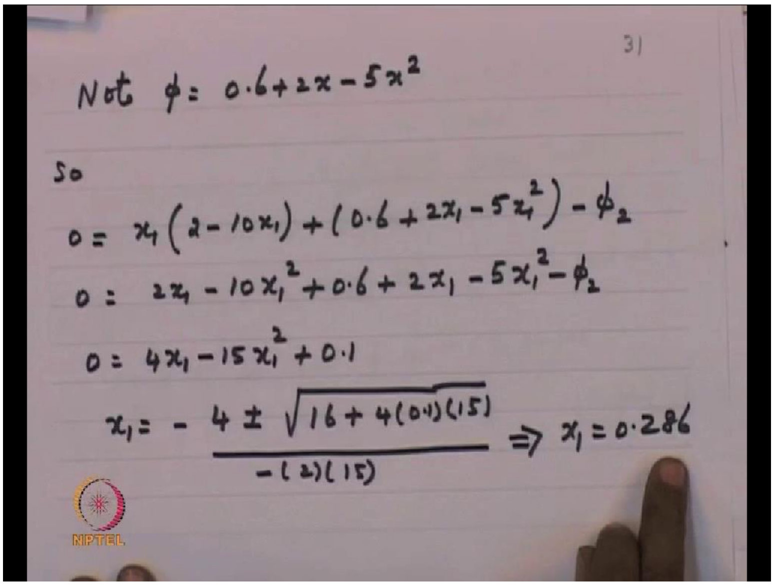

So, I put all these numbers here; 0.286 is correct, now; that means, the highest value for phi we get, when we choose x 1 as 0.286. What is that value? The question now is what is the overall yield?

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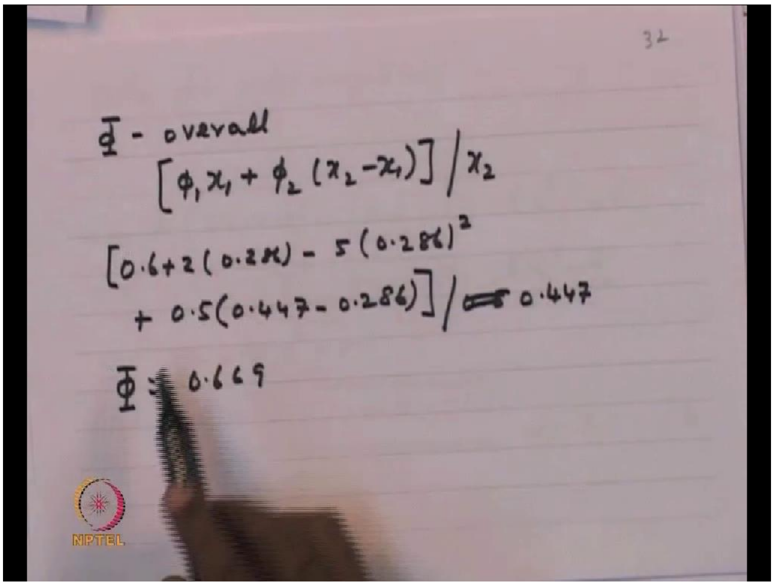

x 1 is 0.286; x 2 is given as, what is x 2; 0.445, whatever that number. This is what I got. So, I get totally, 0.669. Please see, if it is correct. phi 1 x 1; x 1 is 0.286; phi 1 function is given, and then phi 2 times of x 2 minus x 1, which is given here; is it OK? You get 0.669. That is what I get. So, what is so complicated about this calculation? What are we saying is that if we have a two tank sequence and the best choice is to maximize the overall yield function with respect to that intermediate point; that is the point being set.

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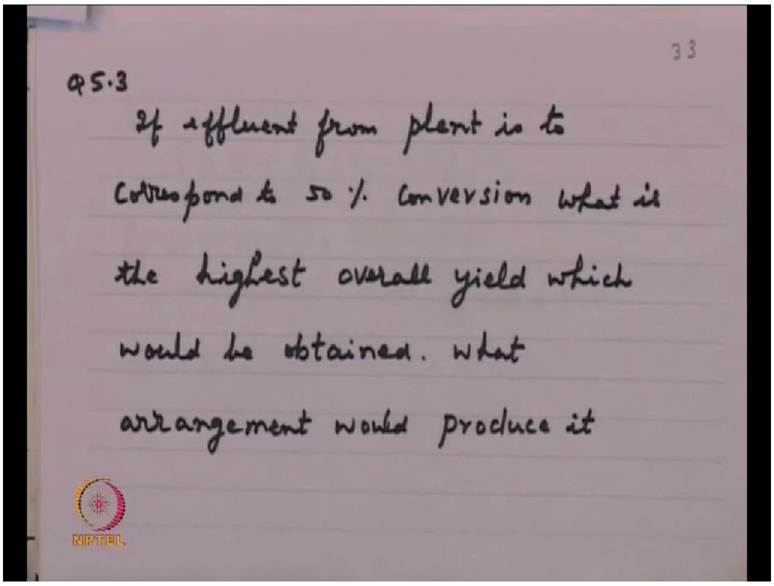

The next result, next point what you want to answer is frequently, in our problem is not just maximizing the instantaneous and overall yield; we also may have some constraints on what is the extent of reaction that we have to reach. I mean, after all, we cannot throw away our reactants, correct; we can make use of them. So, this exercise is about if the effluent from plant is to correspond to 50 percent conversion, which means, we must make use of 50 percent of the material. What is the highest overall yield, which can be obtained? Is this question clear? So far, we were concerned only about maximizing the overall yield. Now, what is being said is that; no, there is another aspect, which is important is that we want to make at least, 50 percent conversion is required. So, what is the max highest yield that you can get? If you want achieve 50 percent yield, what is the highest yield you can get? Let me just state this in a slightly, different way. What is being said is the following.

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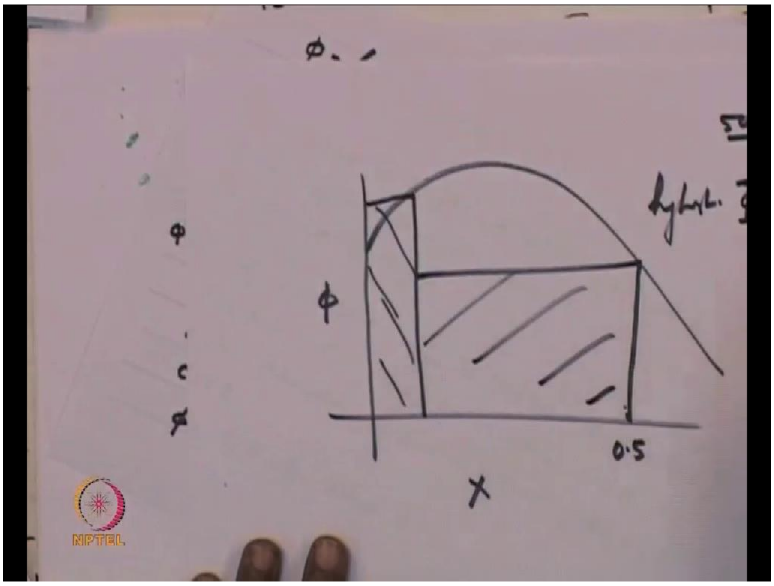

You want to choose a reactor; we do not know what reactor to use. You want to choose a reactor, such that the overall yield, conversion should be 50 percent, we should, and then what is the highest overall yield we can get; that means, you are going to stop at 0.5. This is fixed; our conversion is 0.5. We have to choose the reactor system, so that, the area under the curve is the highest; is that point clear? We have to stop the system at x equal to 0.5, but now, we have to choose. What reactor can we choose? Let us do a small experiment. Let us say I do one here. So, what is the area? This is the area, correct, yes or no? Let us do one more experiment.

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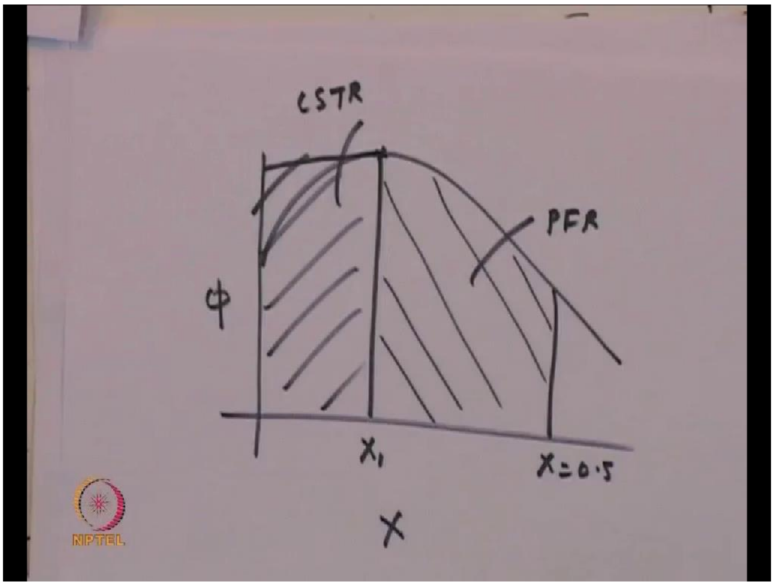

Here, let me; very clearly, if we choose at the maxima, and then here a PFR, is probably be the x equal to 0.5, and this maxima, where it occurs; you will have to find out. This is x 1. So, this will give us the; is this clear what we are saying? So, this is the PFR and this is the CSTR. So, in this case, this is phi and this is x. So, what we have tried to say in this exercise is that when we have a reactor or process development problem, frequently, this procedure would be extremely, right, because you can construct a stirred tank and therefore, construct this curve, phi versus x even, if it is a very complicated reaction.

Once you have this curve in your hand, now, we can play around with how to put your equipment, so that, it will give you what you are looking for. There might be instances where, this curve will go like this, and you are forced to go up to x equal to 0.9, I mean, because of collision control issues and so on. But this is something we accept nowadays. You know we cannot allow our agents to go into the ground. So, accept all this. So, all the issues related with the reactor design; answers can be found out of this. So, this is the advantage of this procedure, which was developed, of course, long back; very useful particularly, when you are working in a development laboratory.

I will stop there.