Advanced Chemical Reaction Engineering
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Lecture - 16
Reacting Fluids as Energy Carrier

We go on with advanced reaction engineering. Today, we will be looking at some practice problems in energy balance. The problem we would like to take is in any interesting exercises let me just explain the background this exercise. And then we will look at the problem itself.

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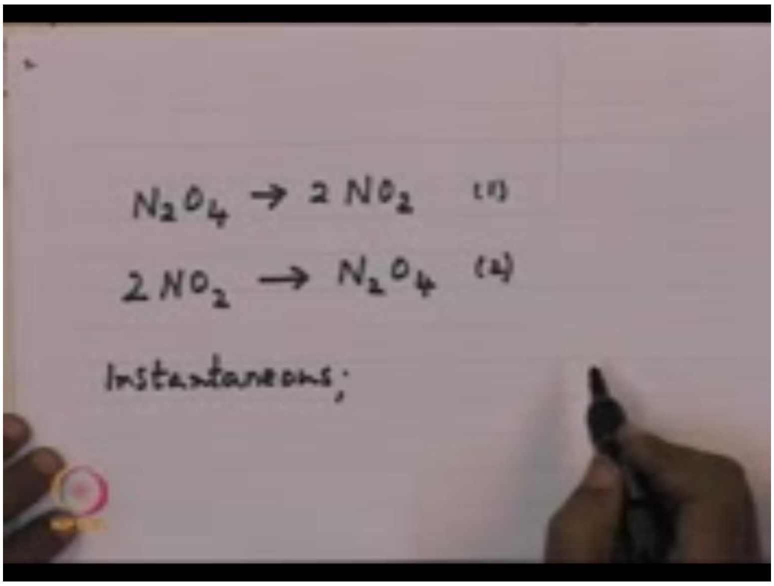

You have nitrogen N 2 O 4 giving you twice N O 2 and twice N O 2 giving you N 2 O 4 so this is the reaction. Now, this, these 2 reactions 1 and 2 the construct with the instantaneous in the sense at any instant of time N 2 O 4 and N O 2 existing equilibrium. Look at some data on this system data looks like this.

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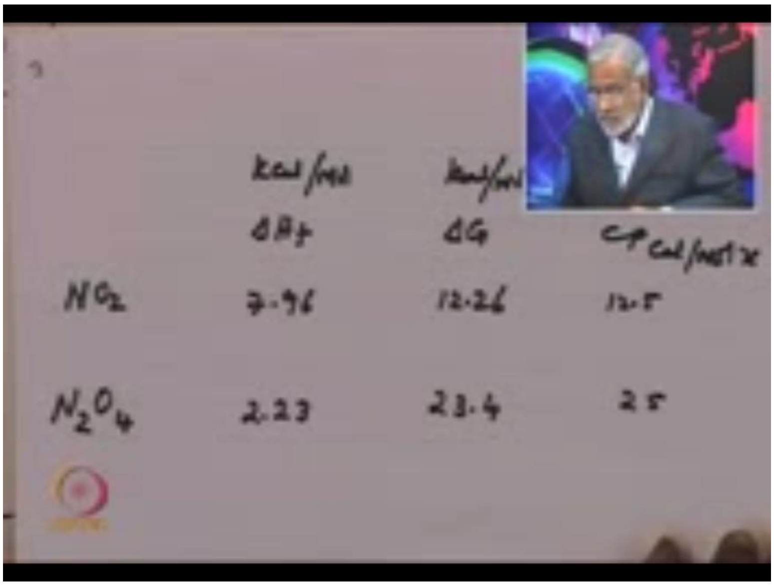

N O 2, N 2 O 4; so, if delta H F 7.96 2.23 delta G 12.26 23.4. C p; specific heat 12.5 and 25 units are k cal per mole; k cal per mole this is calories per mole degree k. Since is reaction instantaneous it is of interest was to see whether we can use this reactions to performs of useful functions. Two functions which are grew interest to society is space heating and of course, production of electrical energy of power. Now, space heating, as you all know if you requires low temperature heat basically. And generally low temperature heat is available this abundance of low temperature heat particularly in the industry. Therefore if we want to do space heating and if we can make use of this low temperature heat then if probably able do in the economically.

Now, if it comes to work of course, we are limited by the first law and we are also to content with the fact that stream which is the working fluid in are engines the power plants. Stream has very large, water is very large vapor pressure therefore, if you want to good high temperatures you necessarily have to good to very high pressures. As a result very high pressure equipment expensive and so on and related has its of etcetera. So, in the, it is in the context we have device this exercise. And to see you know how we can learn to use certain properties of substances that exists around as for some functions that we might think is of we use to it is that is the context. Let us put this context to some use that we are looking at by. Let us see has an example we want to use for space heating application, what is meant by space heating application? Let me just draw what my P T.

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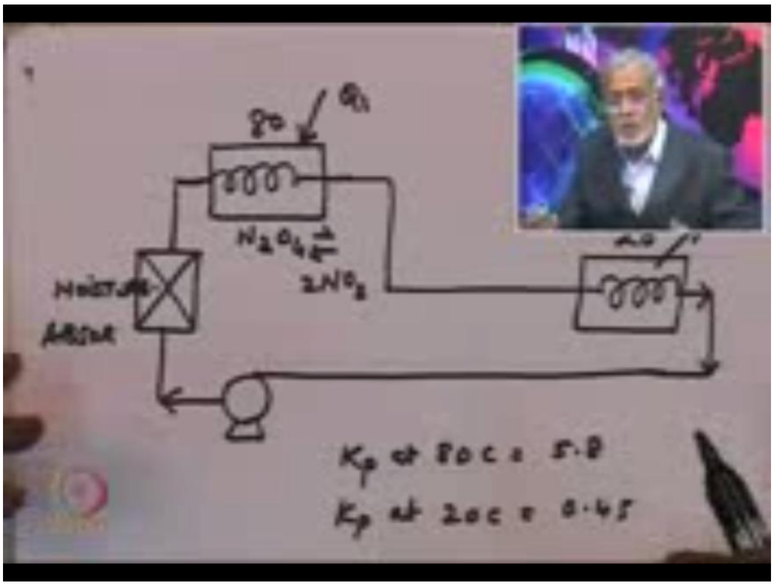

Let us say we have a device so, we have here a so, we have a pump let say this is going from N 2 O 4 going to twice N O 2 N 2 O 4 going to twice N O 2 this is a 80 degree c and this is a 20 degree c. So, material is coming in like this and going out like this. So, what we expect is that it picks up heat at 80 degree centigrade it picks up heat. So, let say Q 1 and then it 20 gives that heat Q 2 and you have a moisture remover moisture. The idea of this moisture absorber is that in case there is some moisture that gets into the system we should get rid of it. Because N 2 O 4 and N O 2 are little corrosive gases we really do not want any moisture at all. So, the essence what we trying to say here is that if you have a device which is able to pick up heat from a low temperatures source.

And this is N 2 O 4 reaction goes towards in the appropriate direction and then here in that this low temperature it is giving that heat. And therefore, it they would reverse that reaction. Now, we get calculate we can calculate based on the thermodynamic that is giving to us let K p; K p at 80 c is 5.8 and K p at 20 c is 0.45. And so what it means is that this reaction at 80 c K p is 5.8 and 20 c is K p 0.45 which means what this is an endothermic reaction. That means N 2 O 4 if it has to go to N O 2 you have to supply heat. And then we derived the temperature the reaction reverses itself it releases heat. Basically it is this a instantaneous ability for this reaction to you know go both ways depending upon the temperature at which the environment is available. It is able to we are able to pick up heat and removed and supplied heat to this source to the environment of are interested.

So, our this whole exercise is to be to be quantitatively evaluate what is the ability of working fluid like N 2 O 4, N O 2 to work as a means of recovering heat from a low temperature source and supplying it towards from a source at 80 and supplying it to a consumarate 20. The consumarate 20 is space heating application is source 80 degree c might be a source of a waste fluid that may be available in an environment may be a factory and so on. So, this is the application that we are trying to evaluate in this exercise. Now, how do we actualize this in a process? Of course, you have to actualize is actualize to actualize this, what is just a days.

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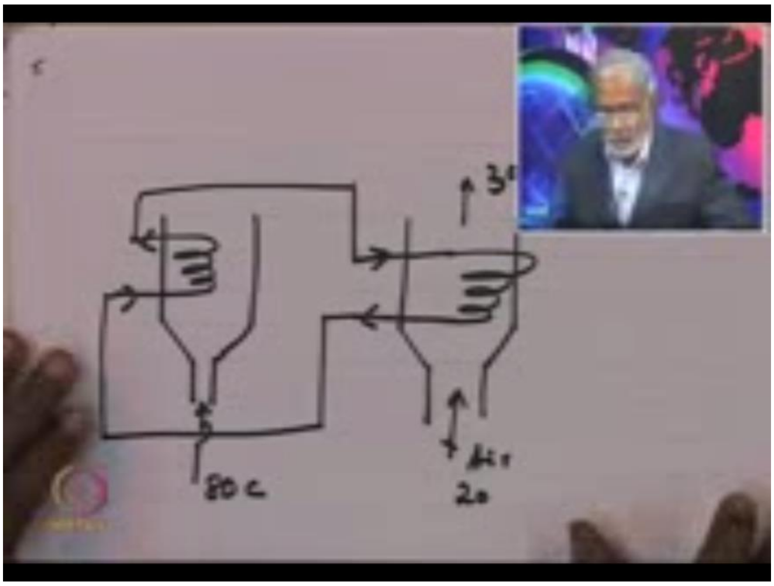

You have 2 fluid beds and you your fluids are moving between. So, you have and its coming in going through like this once second going through that this. So, it comes out like this and goes in like this in comes out like this. What other words, what you saying in that we have, we have a hot this is a, at 80 and this is the so this is come outer 20. So we have let us say air available at 80 and we contact that with this, this coil this quail where 80 degree c temperature is taken up by this gases N 2 O 4 quail to N O 2. And then that is released to air this, another air stream and 2 so that you know 20 if it is 20 will proudly go out at 30. Let us say so that air gets heated and that is how we realize this phase heating application. So, let us module this there are 2 environments this module like this there are 2 environments.

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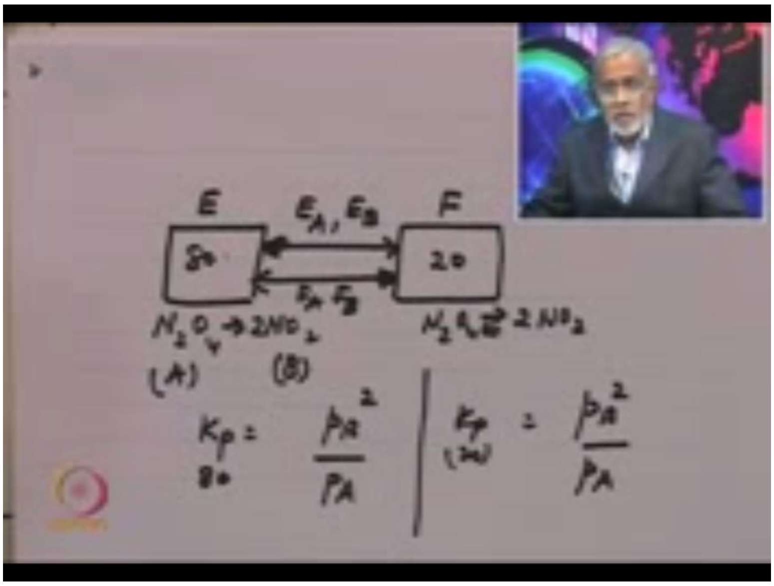

Let us say environment 1 and environment 2, environment 1 is the 80 and environment 2 at 20. You have fluids moving between the 2 by the reaction N O 2 4 giving you to N O 2 takes place both cases it is the same reaction taking place twice N O 2. I call this environment as E and this environment as F therefore, you have so it is going like this so it is E A I will call it E A and E B added I call this is A and I call this is B. And then F A and F B are coming out so, what is the system at we have an environment in 80 degree c which we call is E? And we have another environment is 20 which we call as F and we have this fluids which contains N 2 O 4 N O 2 and so on. We call this E A E B is what is going from E to F and as to and count the low temperature immediately the reaction a takes place. So that the composition changes at F A F B come out.

Now, since the reactions are instantaneous what is that mean? That reaction is instantaneous it means that K p equal to P B squared divided by P A this equality applies. We all understand this from thermodynamics that if the reaction is instantaneous. The compositions of the leaving streams E A and E B will be at equilibrium corresponding to 80 degree centigrade. Similarly, we can say this is this is K p at 80 similarly, K p at 20 also equal to P B squared divided by p and this equality whether its 20 and 80 should whole, because this reaction is instantaneous. Therefore, the composition of the streams must be corresponding to the equilibrium our interest. Of course, is to use this reaction and requires in energy so, we need energy we need what is called as to understand what are this flows E A and E B so, in this particular case.

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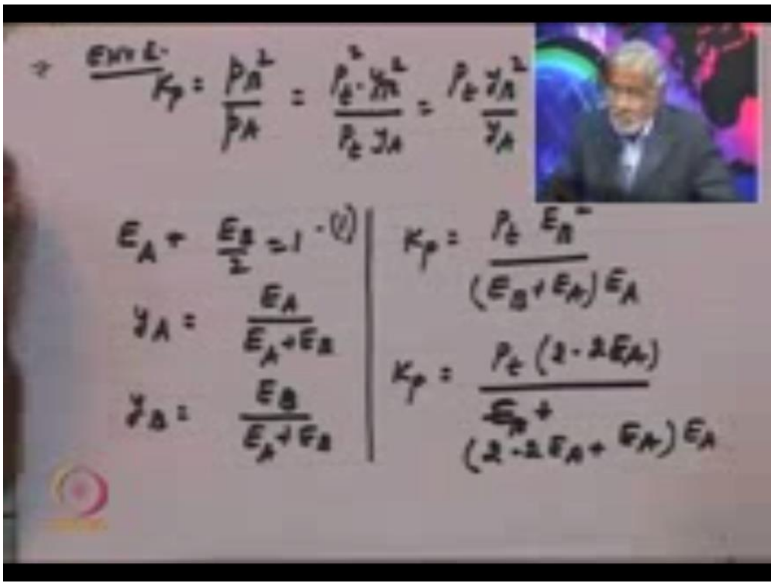

What is mentioned that E A it’s says therefore, the problems says that the nitrogen that is flowing in this stream. The amount of nitrogen here whether it is E A and E B F A F B total amount of nitrogen is 1 mole It is 1 mole per second the total amount of nitrogen that what is specified. Now, we know that we look at E A if you look at stream E A here this stream E A; this stream E. And may coming out the equipment E it as this is this is an N O N 2 O 4 and this is N O 2. Therefore, the amount of nitrogen here if an every mole of this contains 1 mole of nitrogen, but every mole of this contains half a mole of nitrogen. So, if E A and E B are the mole of flows coming out an environment E then what is given to as E A plus E B by 2 is 1.

So, what is the problem statement? Problems state at we have 1 mole per second of nitrogen flowing in the circuit. That means what I am saying that this 1 mole of nitrogen it can be partially is N O 2 depending upon the conditions of the environment. But the total nitrogen the system is fixed which is 1 mole per second so 1 mole per second is accumulating, but as it leaves E that mean environment E. Then will be certain composition of N 2 O 4 N O 2 while it leaves F than be the different composition N O 2 N O 2 N O N 2 O 4. This reason that the temperature is 80 degree and 20 degrees the interrupted composition as determined with the as a different. So, what is y A by definition and what is y B?

Now, we also know that K p I am talking about environment E know K p equal to P B square divided by P A that we know from are basics. Therefore, this P B square what is also can be written as P T times y B square divided by P T y A square so this becomes P T y B square divided by y A. So, essentially our equilibrium representation gives you this K p is given by P T y B by y. Now, y B and y A can be replaced from here so we suppose I do that we get K p equal to P T E B square divided by E B plus E A divided by E A when we are looking at environment E. So, let us do at environment E first and then do the environment F so K p equal to P T y B square is coming from here E B squared E A plus E B whole squared nominated y A also E A. So, it is how so 1 E B plus E A can so we get this type of equation I can simplify this further by writing P T into.

We notice from this equation suppose they are called this as some equation one you can see here from E B can be put from here as to E A to minus 2 E A. I will put as to minus 2 E A that is E B that is E B comes to equation 1 divided by E B, E B plus E B E B is what E B is let be the write this like this 2 minus of twice E A plus E A is it. And replace E B plus E A like this and multiplied by E A equal to K p, is it clear? What we say, what did you say? Let me just run through this whole thing one second we have 2 environments one at 80 and one at 20. The reactions N 2 O 4 2 N O 2 is instantaneous therefore, the composition of this mixture 8 will determined by its equilibrium. Similarly, compositions of this mixture 20 will determined by its equilibrium we will be constant at 80 and 20 are given.

We want to since both this environment are well mixed so we are say are saying that K p value which is P B square by P A which can be expressed in the term y B and y A and so on. Therefore, they are able to expressed the K p in terms of total pressure and mole fractions and mole fractions a of the y A and y B. It comes from basics we also know from the problem statement that 1 mole per second is circulating in the system. Therefore, E A and E B equal to E B equal to 1 y this word half this coming is because we notice that that N 2 O 4 1 mole of nitrogen. While N O 2 is half mole of nitrogen that is y when we say 1 mole of nitrogen is circulating in the system. It means that E A plus half E B is 1. So, that is why we have got this equation 1 alright. So, this equation which you got P T multiply by all these now involves only in E let me this so our equation for.

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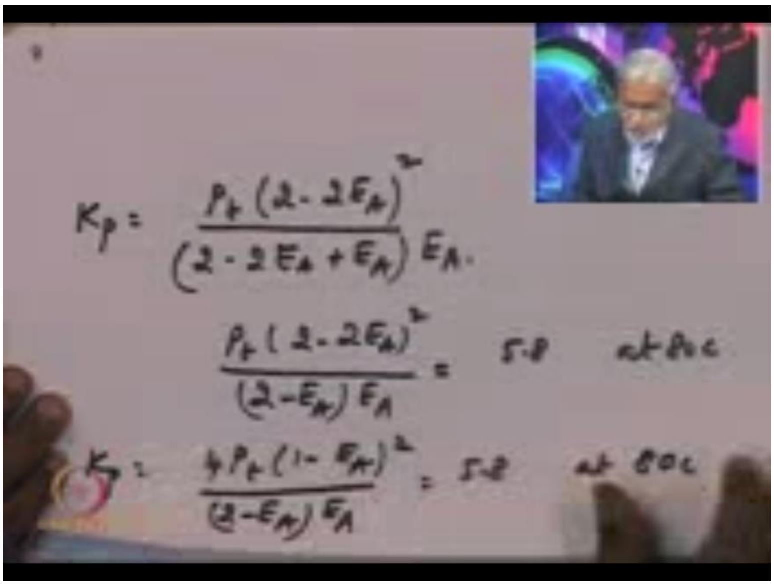

So, K p equal to P T times to minus of twice E A divided by 2 minus of twice E A plus E A within bracket of E A. Or it is P T times 2 minus twice E A divided by 2 minus of E A times E A equal to K p which is equal to 5.8 at 80 degree centigrade. Let me just go through this a it is squared be sink here a squared be sink here squared which sink here is notice is E B squared which is the forgot squared. So, it can simplified further equal to K p equal to 4 P T into 1 minus of E A whole squared divided by 2 minus of E A multiply by E A And that K p is 5.8 at 80 degree c. Now, this quadratic in can be is solved it is see how this solution look likes so it is expand this and simplify when you do it.

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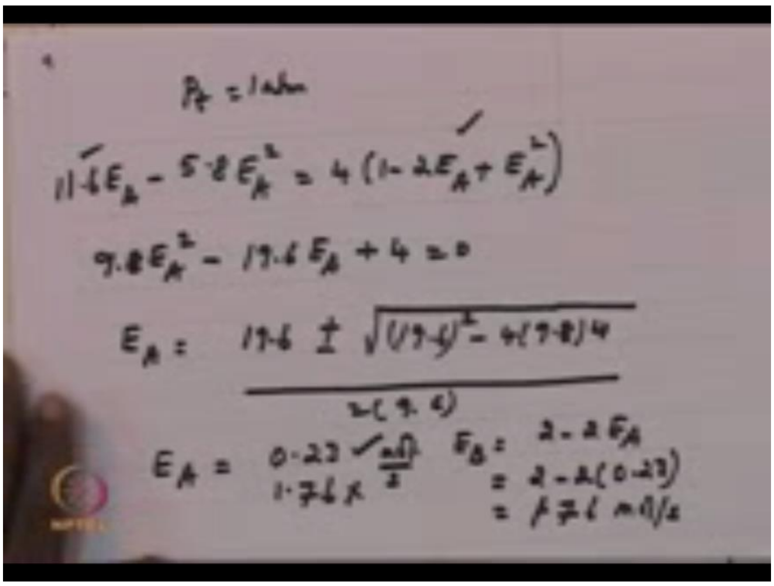

You get 11.6 E A minus of 5.8 E A squared equal to 4 times 1 minus of twice E A plus E A squared. Let me just check how it looks like? 1 minus so this is 1 minus E A squared. So, we have expanding this so when you do that you get this term is correct. And now, 2 E A divided by now it is 2 multiplied of 5.8 is 11.6 that is mix make sense and then 5.8 E A that also make sense. Everything seems alright so, essentially if you we have as of course if taken P T is a total pressure equal to 1 atmosphere that is an assumption. So, this is fine so basically expanding multiplying cross multiplying and then simplify so it is fine. So, we have here so in let me so it is 4 9.6 E A squared, is it correct? 4 9.6 E A square minus 8 E A and therefore, minus n minus 8 19.6 E A so, I have taken this also plus 4 equal to 0.

So, what is the solution? So, E A equal to 19.6 plus or minus root of B squared is a 19.6 whole squared minus 4 times 9.6 times 4 divided by 2 into 9.6 at this 9.8 9.6 E A squared while 9.8 fine. So, this use the solution E A equal to what is E A equal to 0.23 are 1.76 this is 2 solution we get E B equal to minus of twice E A. Therefore, that gives you 2 minus of 2 E A now if you put this 1.76 here the E B becomes. Therefore, this solution is not admissible therefore, the solution is admissible is this second one to into 0.23 that is equal to 1.76. So, mole per second so E A this solution is that admissible so many mole per second.

So, what have you done? What we have done is we have taken this exercise to 80 degrees and 20 degrees we recognized that this reaction is instantaneous therefore, the composition that disclaimed this equilibrium at 80 degrees. And based on that and then the condition that 1 mole is circulating with the system which means that E A plus half of E B equal to 1. So, we put that condition and then through the materials balance to find out what is the value that is appropriate? So, this is as far as E an environment is concerned. So, we have to repeat this for an environment F, because what is this situation in environment f? So, this is environment.

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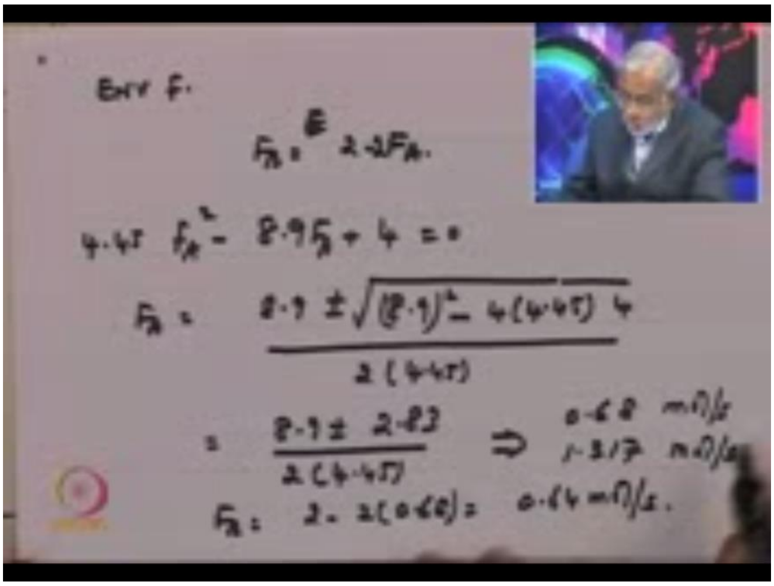

Environment f; what is the situation env f? We have K p equal to 0.45 equal to P T times P T times P B squared sorry P B squared divided by P A. So, this 0.45 so 0.45 equal to P T multiplied by y B squared divided by y A. And now that is equal to y B you can substitute for y B in terms of F A and F B and so on. So, let us do that we have done that already so do it again so our K p equal to 0.45 equal to K p we look like we can write the whole thing one second are equations. Now, will go 4 P T within brackets of 1 minus of F A whole squared divided by 2 minus of 2 F A multiplied by F A. So, it be identical what we got be 4 there it is 4 P T 1 minus E A square here it be 1 minus F A square denominated 2 minus 2 E E A to 2 minus 2 F A so, it is the same kind of an is similar.

Now, then we can cross multiply and simplify and so on when we do that we get 0.9 F A minus 0.45 F A square equal to 4 times 1 minus twice F A plus F A square. Let us see where we got it right so 0.9 so this is a 2 multiply 10.9 F A alright so, it is one second 0.9 F A 0.45 twice this 0.45 F A 2 minus of 2 2 F A and you made missed out plus F A is that so fine. So then F A had missed out so, that is mistake so, 2 minus of F A so, it’s simplifies as 4.45 F A squared minus of 8.9 F A plus 4 equal to 0 let me see this is correct. So, 4 2 8 F A if you take it to this side 8 minus of 0.9 1.9 F A so it is 0.8 minus of 8.9 is at 8.9 correct. This term is correct; this term is taken; this term is taken now, 0.45 F A square 4 plus 4 F A squared this fine and then plus 4.

So, this is the equation so, let as look at the solution to this so the differentially equation this is one second we are an environment, environment F. So, our equation is 4.45 F A square minus of 8.9 F A plus 4 equal to 0. Therefore, F A equal to therefore, F A equal to minus p plus or minus be squared noise minus of 4 into 4 0.45 into 4 divided by 2 into 4, 0.45. So, this the solution and it terms out it looks something like this 2.8 3 divided by 2 multiplied 4.45. So, that gives us 2 solution 6.68 and 1.317 mole per second and we also know that F B equal to 2 minus 2 F A.

So, this is F A therefore, F B equal to 2 minus of 2 times F A if it is 0.68 it comes to 1.32 so 0.68 is that right so, it is F B so, it is 2 is 1.36 0.64 mole per second. And this solution is not that admissible, because 2 times becomes it violates the simple that. So, we have what we have done is that by setting out the questions and equilibrium. We will able to determine the value of E A and E B and this look at the system once again so that understand what we have doing. What we have saying now is based on the thermodynamics of the system that we have, we have F A and F B. This, these numbers are this is 0.64 F A is 0.64 sorry F A is 6.8 and F B is 0.64 and E A 0.23 and E B where is E B and is point to 3 E B and 1.76.

So, we can add up the 2 A plus E B so, if we divided this by to its 0.88 and it comes out to both ones some calculation is take that not exactly one. So, what we I saying is that once impose the condition that they are equilibrium that instantaneous at 80 and 20. And assuming that they are well mixed (refer time: 30:48) is and therefore, the composition is they exist is same composition the inside the equipment and so on. We get value for E A E B F A and FB that they now the question that is the interest was is to find out what is the amount of energy that we can get out it? So, it do this what we have do is we have do energy balance that is do that so, we have the energy balance.

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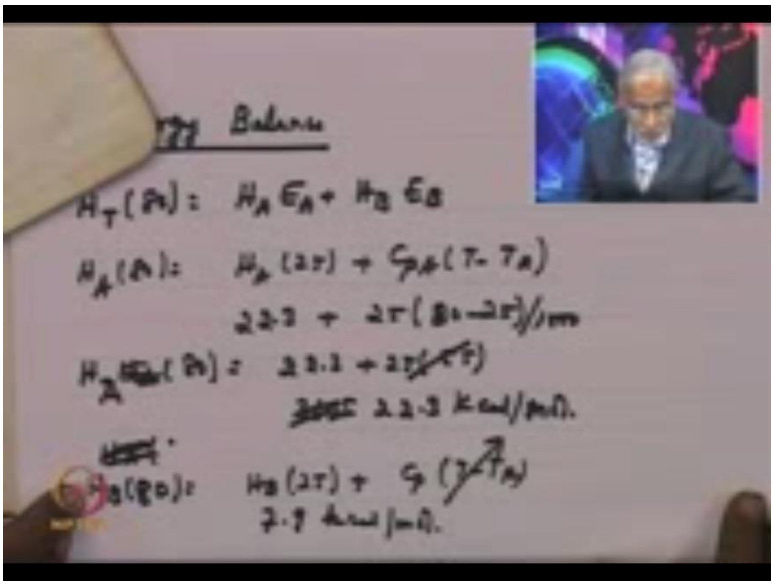

What is your energy balance? We say that the enthalpy at 80 equal to H A E A plus H B E B that means the enthalpy of component A multiply fluoride of component A enthalpy of component B multiple as component B. Now, we have to just calculate what is H A and 80 equal to H A at 25 plus C p into T minus T r. So, this is from the data which is given as 22.3 plus 25 multiplied by 20 multiply by 80 minus 25, is it clear? Because component the environment is at 80 so this becomes so H A at 80 equal to 22.3 plus 25 into 80 minus 25 minus 55. So, it becomes 3605 this is does not make sense? What is 25? 25 is what? What will be units of this? Check the numbers with is units properly taking in care it is calories per mole by all these are in kilo calories.

So 22 H A is 22, because the, and this is calories per mole so it 0.1 to 5 so it is divided by 1000. So, this is not important quantities so it is something like 22.3 kilo cal per mole H A 80. Similarly, we have to find out so what is the total this is the H component at 22.3 H component B at this is for component B at 80 degrees is H B at 25 plus C p T minus of T r as small quantity is neglect this not will be in important quantity H B is the 25. We can calculate the data has been that is given to as H B 25 the date is given to as here 23.1 and 2.23 sorry 2.23. And so that comes out to from the data it times of 7.9 it is 7.9 kilo calories per mole. So, what we have done? We have calculated what is the enthalpy of component A what is the enthalpy of component B? Therefore, we can now calculate what is the energy that is associated with the n as to that what is the energy associated is stream? What is the energy associated with this stream and is straight forward energy associated with the Total amount of N g at the environment 80 is an E A H A plus E B H B what is E A?

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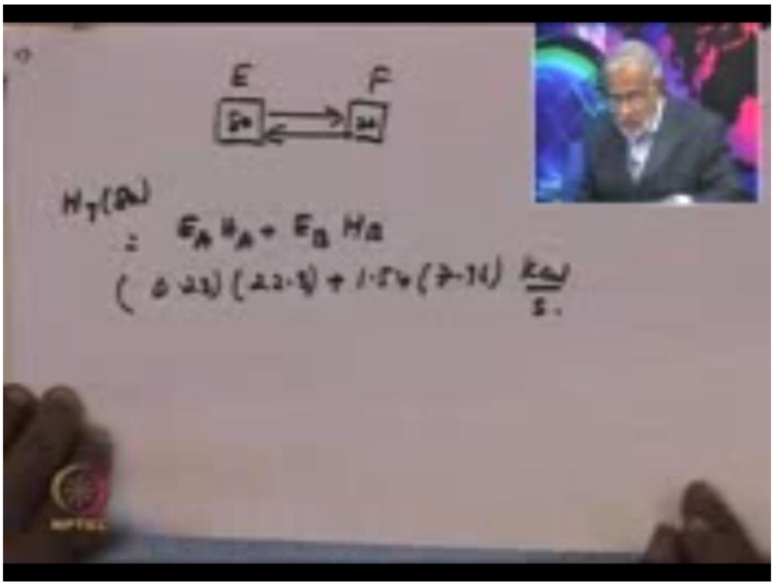

E A is 0.23 multiplied by 22.3. And then E B is 1.54 multiplied by it is 7.96 so many kilo calories per second, is it clear? What we are saying is we know the mole of flows our system is incators system or system is escape the whole. And we can draw it once again this is our system is this is E and this is F. This is going like this coming like this; this stream E A is 0.23; this 0.23 E A is 0.23 and E B is 1.54. So, if we divided this by 2 it is 7.7 so, 0.77 from 0.23 is 1 so enough its satisfies the material. So this is as far as at 80 degree stream is concerned this is 20 so, you want to do this same thing at what happens at 20 we repeated that 20. So, we calculate what is the energy associated with streams and are leaving at the so, for the 20.

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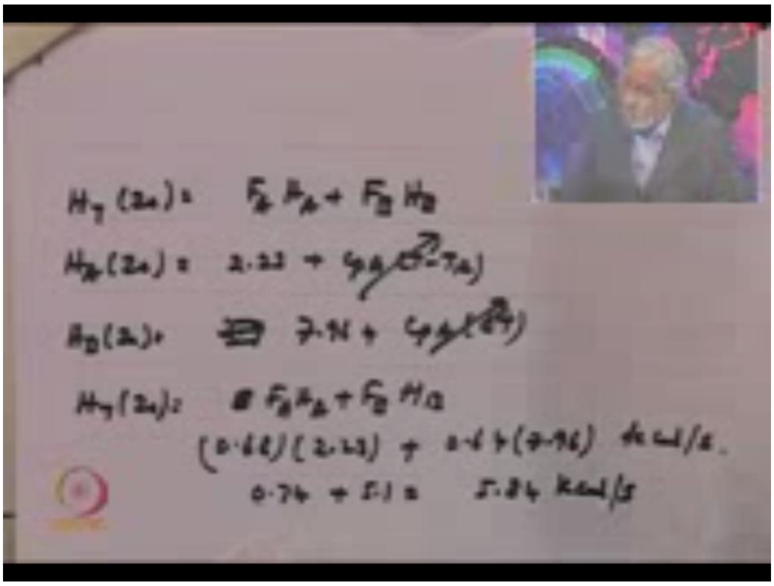

So, H so the total amount of energy at environmental 20 is F A H A plus F B H B this we know. So, H A at 20 we have to calculate that is equal to 2.23 plus that C p terms C p T minus of T r which we will neglect. And similarly, we have H B at 20 equal to 7.96 minus C p that term delta theta will neglect it 7.96. So, our H T at 20 equal to E sorry F A H A plus F B H B So, F A is how much? F A is 0.68 H A is 2.23 and F B is F B is 0.64 multiplied by H B and the H B 7.96 so many kilo cal’s per second. So, this is roughly 2 by 3 so, that is about this about 0.74 this is a 84 point through about 5.1 that is about 5.84 k cal per second. This is energy balance H A H B estimate we want calculate H T.

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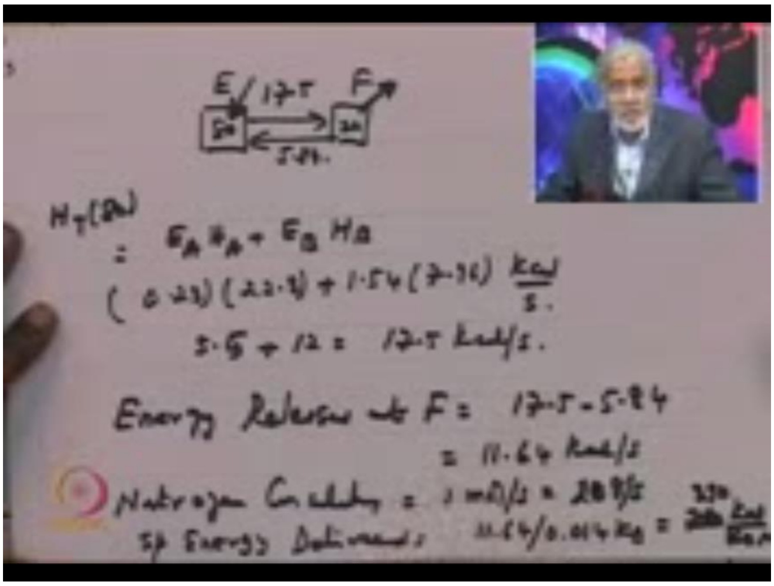

What is H T at 80 by this quickly calculate this that is about one fourth; one fourth of this should be about 5.4 5.5 and this is 8; this about 12 and this is about 17.5 kilo cal per second. So, what we are saying now is the energy that is the energy that is in this stream is 17.5 units the energy that is in this leaving stream is 5.84 units. What are we say? What we saying is that energy that is leaving the 80 degree centigrade environment is the 17.5 units. What is leaving is five point therefore, the energy that is delivered that means what we taken up minus what is this energy that is delivered to be. Therefore, energy released into environment F equal to 17.5 minus 17.5 along with 5.84 this is 5.84 minus 5.84 5.84 that terms are to be 11.5 is about 11.64 kilo cal per second. Now, if I want to calculate this nitrogen circulating is 1 mole per second or 14 grams per second 1 mole is 14 grams.

Therefore, the energy that is delivered to this stream per gram of nitrogen so specific energy delivery delivered is 11.64 divided by 0.014 k g. So, that is about 0.014 is about 7 so about 70 77 so, it is about 780 kilo cal per k g nitrogen. You will understand what are we saying this is an important figure we are being able to transfers 11.64 cal calories per second into environment F so much. A space heating has been provided to do this we had to circulate 1 mole per second of nitrogen of 28 I am sorry 28. So, this is 390 is 390 kilo calories per k g nitrogen so, what this working fluid which is a N 2 O 4 N O 2 System is able to do theoretically. Based on whatever numbers we have generated is that is able to pick up and deliver 11.64 kilo cal’s per second for 1 mole per second of nitrogen circulating 1 mole is 28 grams per second. So, I divided by this 28 028 let do this one second numbers are in our mind, this is an important numbers which may have some implications later.

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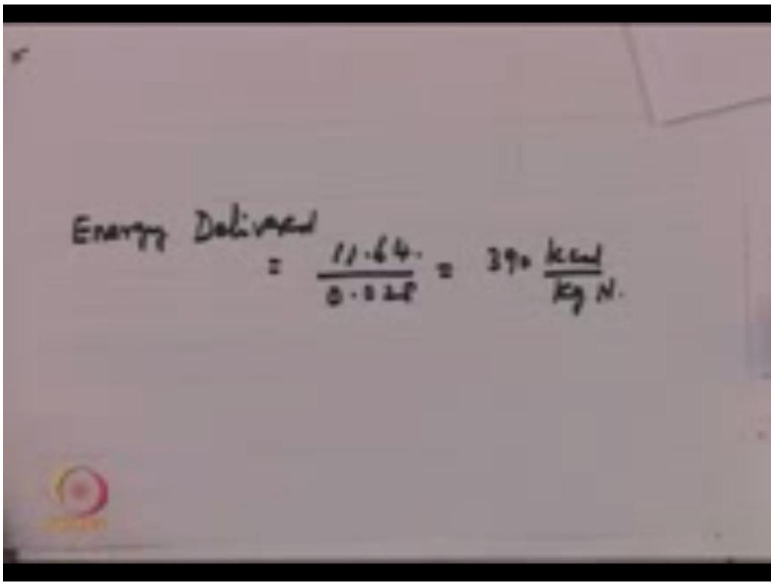

So, energy delivered equal to energy delivered to equal to 11.64 divided by 0.028 that comes to about 390 kilo calories per k g. So, we unable to delivered 390 kilo calories per k g of nitrogen circulating. Now, this, these numbers are a very important vies come to that minute. Now, the context to looking at this should not be forgot the context is of the following N 2 O 4 N O 2 is system in which there is no phase change let me everything is in the gases phase no one. Therefore, we can look at fairly high temperatures may be 120 140 depending upon the kind of low temperature heat that may be available in an environment. So, if you low temperature heat available 120 130 and 40 whatever then clearly if you looking at stream as a working fluid.

Then we are looking at much high pressures so essentially it is the high pressure that is to be handled with stream which makes the use of stream a little expensive. Because of course, stream is not course is not course in great properties and so on but you are go to higher pressure here that features is not there. And second thing which is equally important in that we are able to transfers fair fairly large quantity of energy is not small. As you can see here it is 390 kilo calories per kilo gram. We can do this similar kind of calculations for work also and I want to do that I do that right to way just to go this calculation. So, this not difficult to do I will not give the details so, you we have here if we do the same calculation for work you find.

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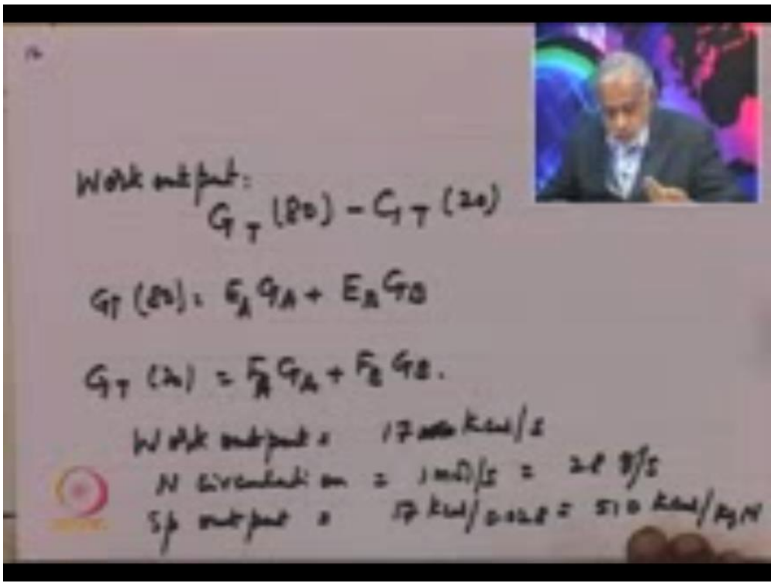

That work output measured as G T that is G and G T at 80 minus G T at 20. That means how do you find G T? G T is calculated as E A G A plus E B G B. Similarly, G T at 20 is calculated as F A G sorry F A G A plus F B G B. Now, G A and G B into calculate G A and G B you should know the, a standard it free energy of form it all that is giving. So I put all this numbers are and got this so when you put in all your numbers. It looks something like this that work output equal to about 17 kilo cal per second and nitrogen circulation is 1 mole per second or 28 grams per second. Therefore, specific output equal to 17 kilo cal divided by 0.028.

Now, 17.028 is something like how much is that 80 forward 3 that is 30 and to 510 kilo cal per kilo gram of nitrogen. If indeed we want to drive and engine between 80 and 20 we get about 510 kilo calories per gram of nitrogen. This is the difference between if we looking at stream to do this same kind of work we find that the amount of work we will get is very very small. Because of variety of reasons one of course that at 80 and 20 the energy there is contain a stream is not large enough. And therefore, the temperature difference is also not sufficient and so on.

So, this to cut this long story short what we have to trying to say here is that if you are using this working fluid which is N O 2 N 2 O 4 working fluid. Then we are able to derive pick up heat from low temperature source may be 80 degree may be 100 may be 120 130. And since it is there is no phase change involved in this system you do not go to higher pressures. And therefore, the huge advantages from the point of a required a heat at low temperatures. So, heat is an instance of a chemically reacting system being used and to pick up heat and delivered heat or to actually pick up the energy and deliver work. This not a very common in a system that you will see in daily life N 2 O 4 N O 2 is highly corrosive.

And therefore, it is not used commercially that, but the point of discussing this here is not so much that is not commercially used. But to point out the fact that if can think of making a synthetic substance which is inert which it got this kind of properties which can be used as the working fluid. And therefore, we do not have that look at stream and there will be a great advantage in as far as commercial and then daily life is concerned. And it would be a great product if we can think of a product life is. That is the context of looking at this example to illustrate how we can use the chemically reacting system to give work on to give heat as may be the case.