Mass, Momentum and Energy Balances in Engineering Analysis
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Lecture - 15
Energy Interactions in Reacting Systems (Contd.)

Welcome, today in this lecture we shall be doing some problems on the Energy Interactions in Reacting System. So, here we shall be using all the concepts we developed in our last lecture and check that how to implement those concepts in solving some real life problems.

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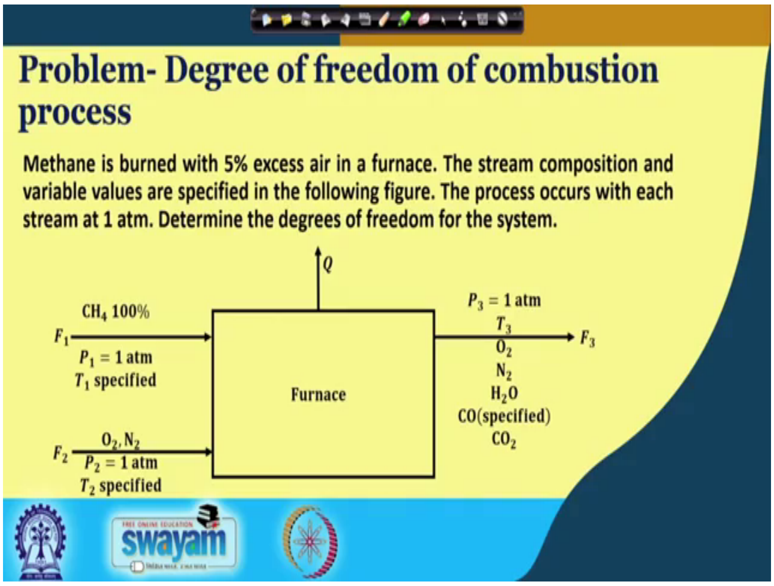

So, first problem is on the concept of degrees of freedom and this has been applied for a combustion process. In this problem methane is burned with 5 percent excess air in a furnace. The stream composition and the variable values have been shown in this particular figure. And the process occurs with each stream at 1 atmosphere pressure. So, we have to determine the degrees of freedom for this system.

So, here you can see, this is a typical representation of the combustion of methane. Here we have a furnace and we are inputting the methane stream and the air stream. And as you can see that air is basically consists of nitrogen and oxygen which are the major components of air. And here the pressure have been written and the temperature will be something arbitrary, but it is specified.

Now, after the methane gets combusted, there could be the production of carbon dioxide. If there is a complete combustion and if there is partial combustion there will be production of carbon monoxide. So, you can see in the outlet stream, we have a carbon monoxide and carbon dioxide both of them and then it will also produce water. So, here we have H2O plus some unreacted oxygen and the nitrogen is remaining unreacted all throughout.

So, whatever nitrogen is going inside the furnace will be coming out of the furnace without any kind of reaction, but what changes will occur is this the inlet streams will be having certain temperatures. Due to the combustion the temperature of the outlet stream will be different from the inlet stream temperature. And here it has been shown the queue; that is if there is any kind of heat exchange between the furnace and the surroundings.

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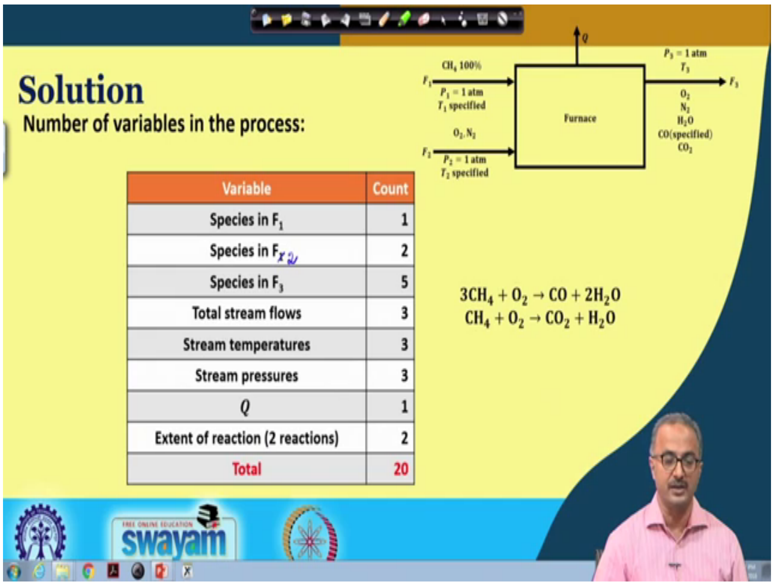

With these information now, we shall be doing the degrees of freedom analysis to figure out whether this problem has been defined from properly or not, so that we can solve for the unknown variables.

Now, first as we learnt that we have to first list out all the unknown variables. So, here you can see that we have listed out the variables. So, species in the F 1 and there is again, I have shown for your reference this particular figure. So, here we have only 1 species, so that is why we are counting only 1. Then species in F 1, this will be F 2, so this will be

F 2 here, ok. So, this in F 2, we have 2 species that is oxygen and nitrogen. So, we are counting 2 here and in the stream F 3, here you can see we have 1 2 3 4 and 5. So, we have 5 components and we are putting 5.

Now, please understand what we mean by these species in F 1, F 2 or F 3, we mean that their composition, ok. So, how much of thus, these species are present in each of the streams is given by there may be mole fraction, may be mass fraction, or maybe some concentration in terms of say mole per cubic meter. So, all those things are being counted. So, that is what we mean by this counting of the species.

And next we come to the total stream flows. Now, here we have three streams F 1, F 2 and F 3. So, these are the 3 variables. And then we have stream temperatures. So, associated with each stream there will be one temperature. So, we have 3 streams. So, we have 3 temperatures and then steam pressure. So, we have 1, 2, 3 streams, so, we have this stream pressure. And then the queue that is the amount of heat that is going out of the system, that is the 1 and extent of reaction.

Now we have two reactions possible as I just told you. So, methane can react with oxygen partially to give carbon monoxide or it can also react with oxygen completely to give us carbon dioxide, ok. So, for each of these reactions, we can associate some kind of extent of reaction as we learned in our earlier lecture and this will be counted as 2 more variables.

Now, if you add up all these number of variables then you add up to they add up to 20. Now after counting the variables we have to count the number of independent equations correlating these variables. So, let us now go for this equation counting.

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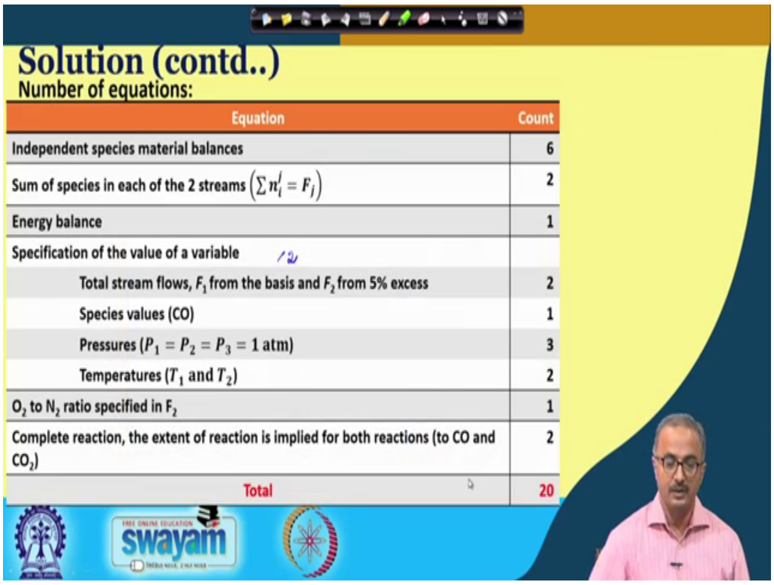

Now, here we have put all the equations that are necessary for this. Now, first we have the independent species material balances, they will count to 6, ok. For each of the species like we can see here that we have 1 plus 1 this methane, oxygen, nitrogen, 3 then water 4, then carbon monoxide 5 and carbon dioxide 6. So, we have 6 species involved in this particular process. So, we are putting that for 6 of this species, we have 6 material species material balances.

Now, once you are writing the species material balance there is no need to write the overall material balance, ok. Now sum of species as I was telling you this will be counting to the total stream flow. And for these two streams we are having this total stream flow. Energy balance will be always be 1, because energy balance is not done species wise, but it is done for the overall system so, it will always be counting to 1 and then specification of the values. Now, you understand this, these specifications if you do not make these specifications; that means, you can also do the degrees of freedom analysis without these specifications, ok. So, if you do not count this then you will find that this total count will not be so.

Now, when you specify what we are trying to do is that you are trying to reduce the degrees of freedom to 0 so, that you can get some unique solution, ok. So, that is why we are doing this specification count. So, here we have some specification please, understand that the specified variables are not unique. The selection can be a user based thing depending on the situation the specifications can differ, ok. So, this is one of the typical set of specified variables, I can say depending on the situation you can also alter this set of the specified variables, ok. For this particular set as you can see that we have specified the pressures temperatures, etcetera and this oxygen to nitrogen ratio in the feed stream. And we are assuming complete reaction to extent of reaction is implied for both reactions, etcetera.

So, all these things you will find that we have specified these variables, ok. So, if we specify this sort of variables and then we count these equations then what we find we are having these 20 equations. Now you can see that when we are doing the degrees of analysis. Now, we have to simply count the number of variables, number of, independent equations and then degrees of freedom means 20 minus 20 that is 0. Now 0 means we have a unique set of solution, unique set solutions for all the unknown variables in the problem.

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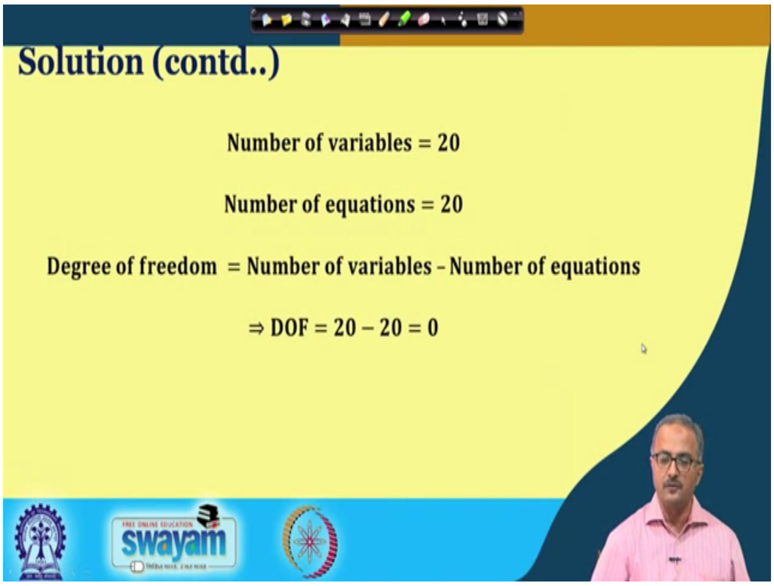

So, every time what whenever we want uniqueness, we have to make sure that the degrees of freedom is always 0.

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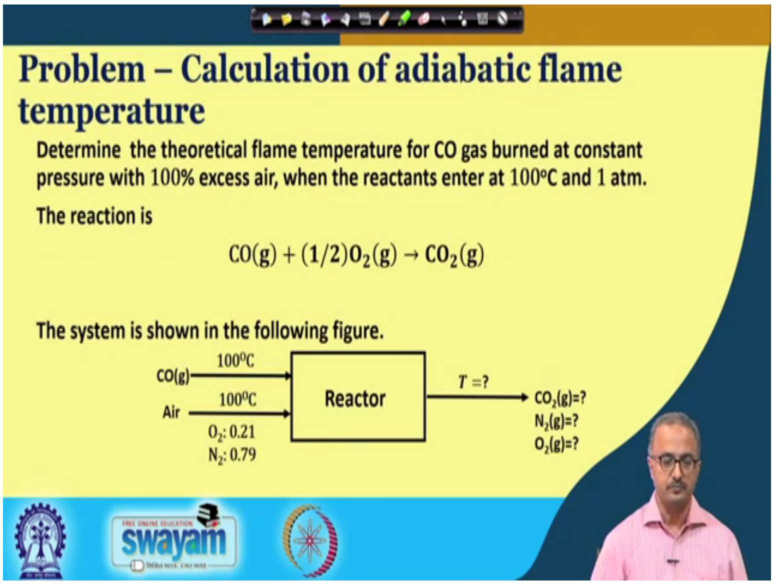

Next, we come to another problem. In this problem, we have to estimate the adiabatic flame temperature, what it means is this whenever there is some kind of combustion happening. Now due to this combustion, you know that it will lead to some energy generation and there will be rise in the temperature. So, this rise in the temperature can be estimated and there can be are various methods.

Now, in adiabatic flame temperature, it means that word adiabatic means that it is assumed that there is no heat transfer between the systems and the surroundings so that whatever heat is being generated by one particular reaction that remains within the system. So, that heat can increase the system energy or internal energy of the system to the maximum possible extent, ok. So, that is the significance of the adiabatic flame temperature.

So, here we have to determine the theoretical flame temperature or adiabatic flame temperature for carbon monoxide gas burned at constant pressure with 100 percent excess air when the reactants enter at this temperature and this pressure and this is the particular reactions. So, this is the Stoichiometric reaction which is given in terms of that for 1 mole of carbon monoxide getting combusted with half a mole of carbon oxygen to give 1 mole of carbon dioxide all in the gaseous state.

Now, please understand that whenever we are doing this kind of analysis, we are assuming that the outlet temperature pressure of the exiting stream is same as the reactor temperature, ok. So, that is why we are not counting the reactor temperature and pressure separately. And the same thing we did in our earlier problem too, we did not count the temperature pressure of the reactor separately from those of the outgoing streams, ok.

Now, here we put all the conditions as given in the problem. And here we are assuming that the air to be a binary mixture of nitrogen and oxygen, ok. Even though air is not truly binary, but here we are assuming to true binary mixture. And in that case, we take that conventionally, we take the air to be composed of 79 mole percent of nitrogen and 21 mole percent of oxygen. So, when you convert the mole percent into mole fraction, you get 0.79 mole fraction of nitrogen and 0.21 mole fraction of oxygen.

Now, here we have to find out the temperature at the outlet and also we do not know the composition of the outgoing streams. Only thing is this, we know that this nitrogen which is going into the reactor will come out fully without any kind of reaction.

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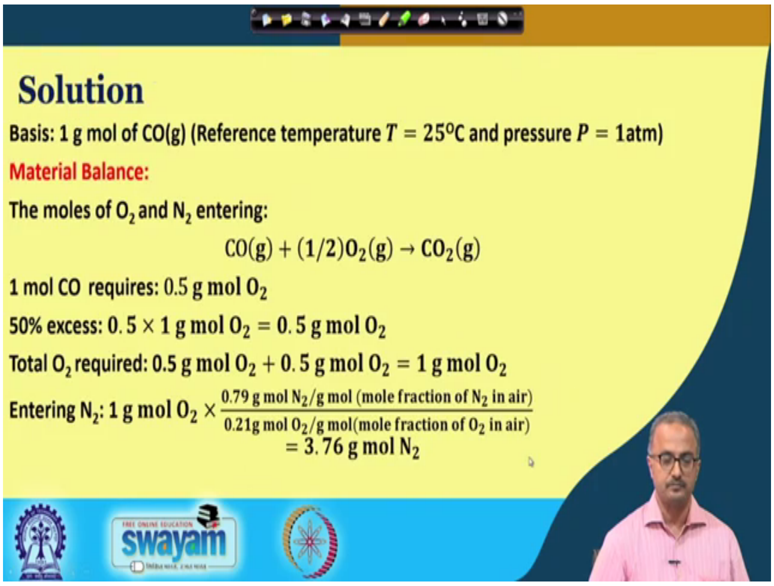

Now, what we do that as we learnt earlier we choose a basis. So, here we are choosing a basis of 1 gram mole of carbon monoxide as our result in the problem statement is to be reported in terms of this particular quantity, ok. And the reference temperature is taken to be 25 degree centigrade and pressure to be 1 atmosphere, because as you know that the enthalpy is to be found from some reference values of pressure and temperature. So, these are the two values of temperature pressure based on which we are going to find out the enthalpy.

So, we write the balance equation here. And now what we find that 1 mole of carbon monoxide reacts with 0.5 gram mole of oxygen. And in the problem statement is says that we have sent 5 percent excess so; that means, the actual amount of oxygen sent is the 0.5 is a stoichiometry amount into this 1 gram mole, this is the excess amount of oxygen we are sending. So, total oxygen is this 0.5 gram mole that plus the 0.5 gram mole that is 1 gram mole, ok.

Now, once we know the amount of oxygen sent into the system then we can now calculate the amount of nitrogen entering into the system by knowing the composition of the air. So, here we are writing that for 0.21 gram mole of oxygen, we are getting 0.79 gram mole of nitrogen. So, for 1 gram mole of oxygen how much nitrogen will be sent? So, this is the amount of nitrogen that is also entering the system with the air.

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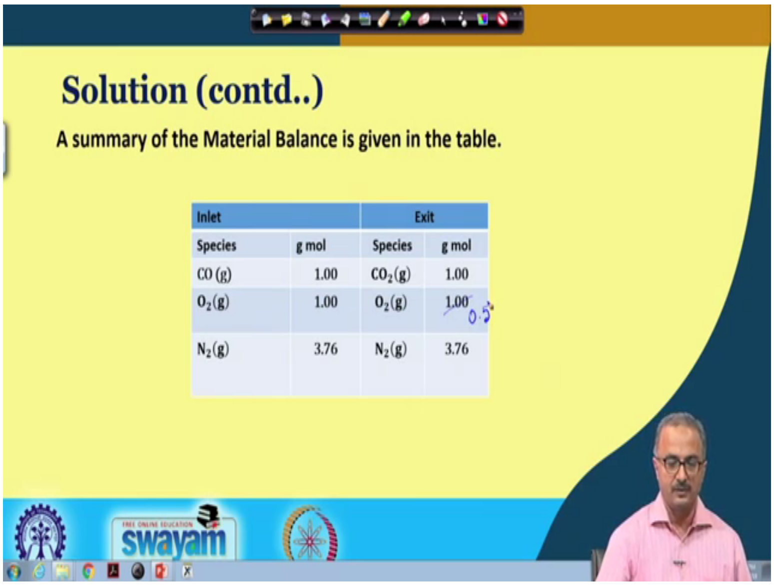

Now, we write the material balances that these are the gram moles of carbon monoxide, oxygen and nitrogen and these are the various species at the outlet. And now from stoichiometry we can know how much of carbon dioxide, how much of oxygen and nitrogen are going to be produced, ok, because we are going to make this. One more thing that in the exit, we have 0.5 gram mole of oxygen, because another 0.5 gram mole has reacted with carbon monoxide.

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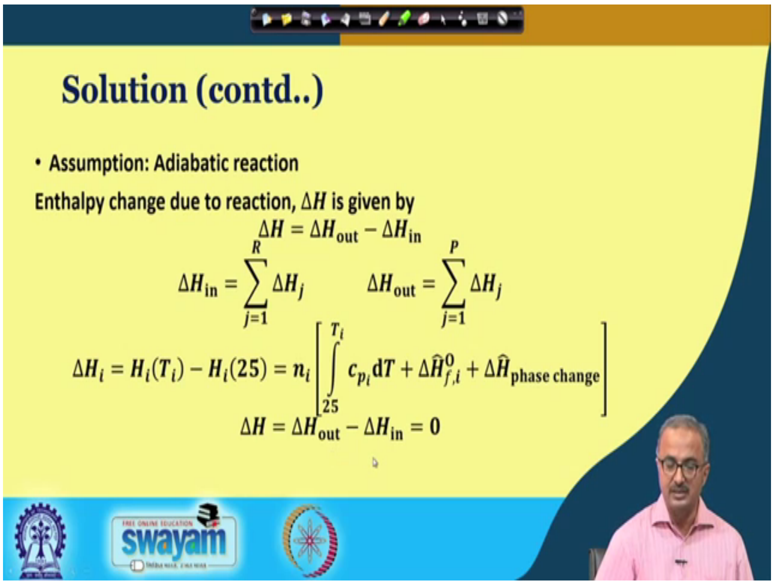

So, after these material balances, now assuming that adiabatic condition now we find out, we have to find out the enthalpy of the reaction. So, that we can find out the temperature and we know that enthalpy of reaction is given by delta H out and delta H in. And in this case the in one we know, because we can find out the total enthalpy change associated with each of the components and here outside also enthalpy change associated with each of the components. So, here this R is representing the total number of reactants in and the P represents the total number of products species.

Now, we know that delta H i equal to H i T i minus H i 25 that; that means, this is the standard temperature for us. So, with respect to this standard temperature, we are trying to find out the enthalpy of, enthalpy change for ith species. And as we have derived earlier that in this case we have to take the sensible heat, we have to take the heat of formation and the heat necessary for the phase change.

Now, the with this particular thing, we know that this is the adiabatic. So, we are putting this delta H equal to 0 that will delta H out is equal to delta H in.

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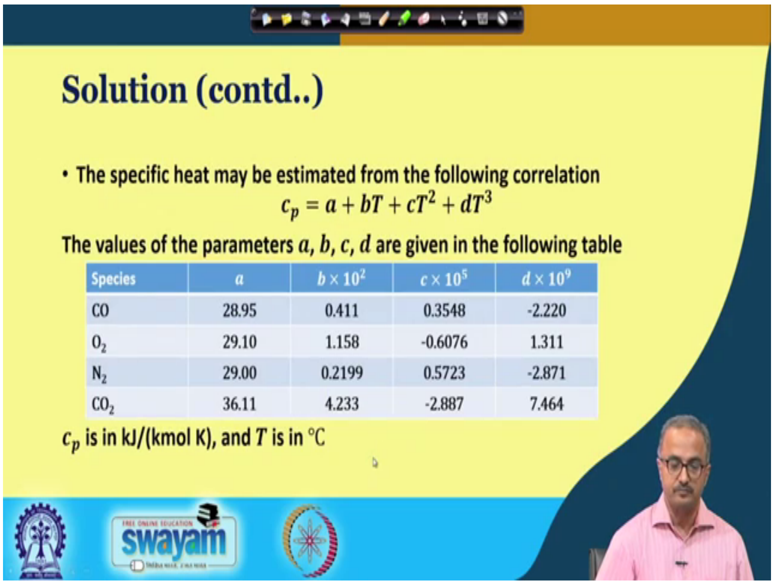

Now, this is what we learnt earlier that C p may be given by this cubic, polynomial and here we have given you the a b c d values for all the species, ok. And here, we say that the Cp is in kilo, joule per kilo mole Kelvin and temperature is in degree centigrade.

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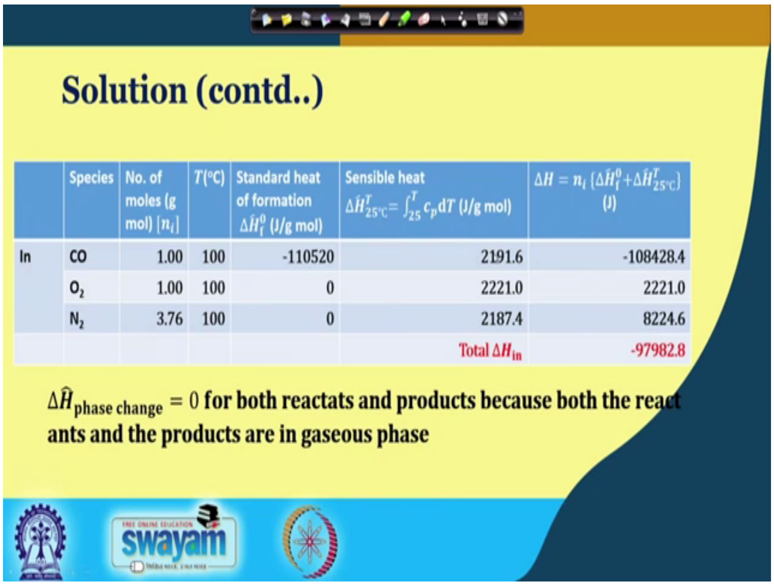

Now, next of the things are very simplified, I am not going into detail of this, because I have done such a calculation in the earlier lecture. So, here we simply put this formula and find out the delta H, this sensible heat from this particular integration. And I have just put the final values after doing this integration here and the total change in the enthalpy. As we learnt earlier has to be found out by multiplying the respective amount of the number of moles of the species with the change in the enthalpy for that species. And for each of the species we have simply multiplied these numbers the number of moles to get all these things. So, we are we are adding these two up and then we are multiplying with number of moles. So, we add this two up and multiply this mole, we add this two and get multiply with this number of moles.

So, after doing this, we are finding this is the total enthalpy change at the inlet stream. And then we know that there is no phase change in the system, because all the species are in the gaseous phase. So, we are putting this enthalpy change associated with the phase changes 0.

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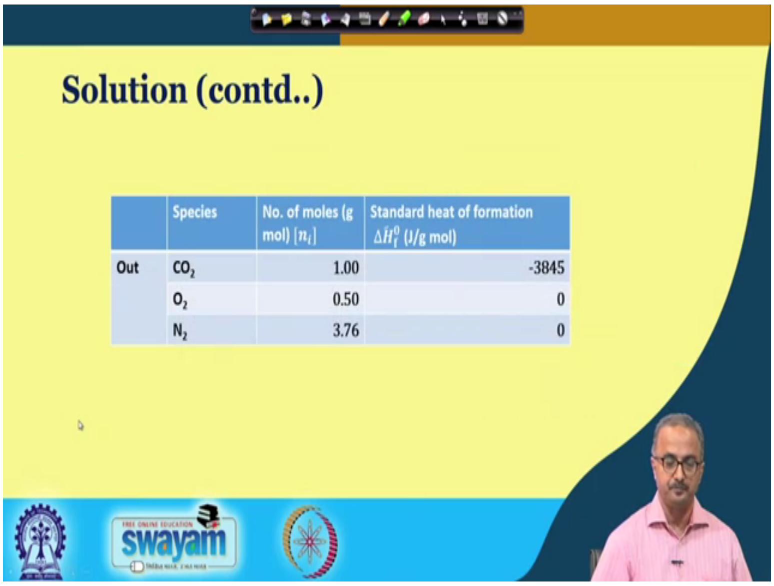

And now, we have all these information about the outlet stream, these are standard heat of formation. And again these values are found from the data chart given in the literature.

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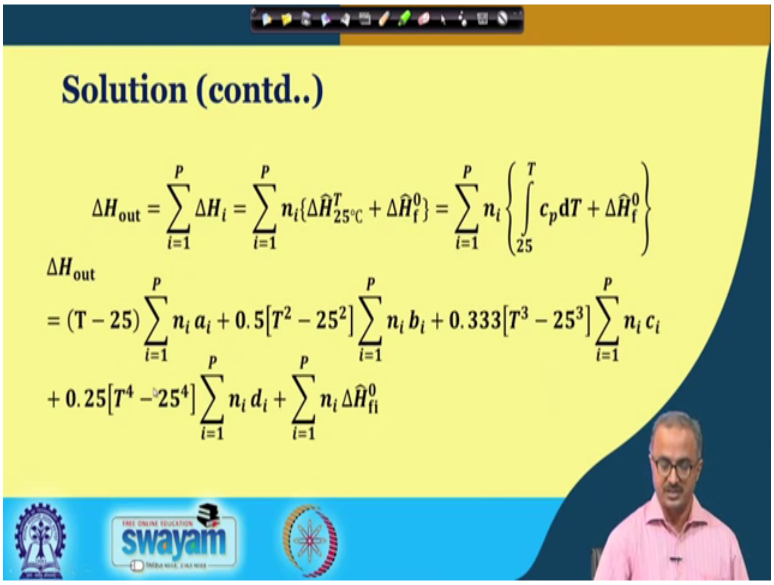

And now, we are ready to find out the delta H out and again we are putting all these. This is the final equation for the delta H out, it is similar to the word that is in, delta H in. And what we are doing now? We want when we add up all these over the species. What we find these all these temperature terms can be brought out of the summation and the summation is occurring for each of the components for each of the parameters in the specific heat equation.

So, here you find all these summation represents the parameter in the specific heat equation and these terms are representing the terms after the integration.

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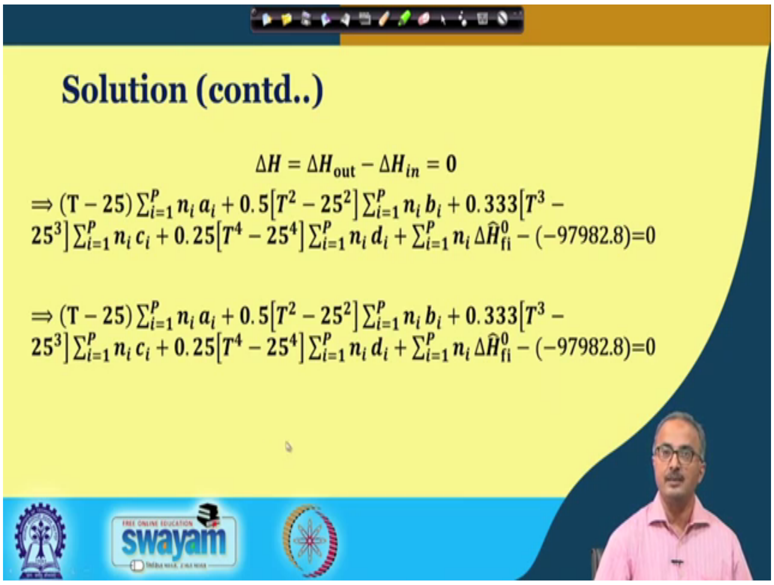

So, here I am not any more going to detail, it is simply rearranging the two equations, we have found out for these two's enthalpies. And next is this, we are finding that the final equation becomes a cubic equation in temperature.

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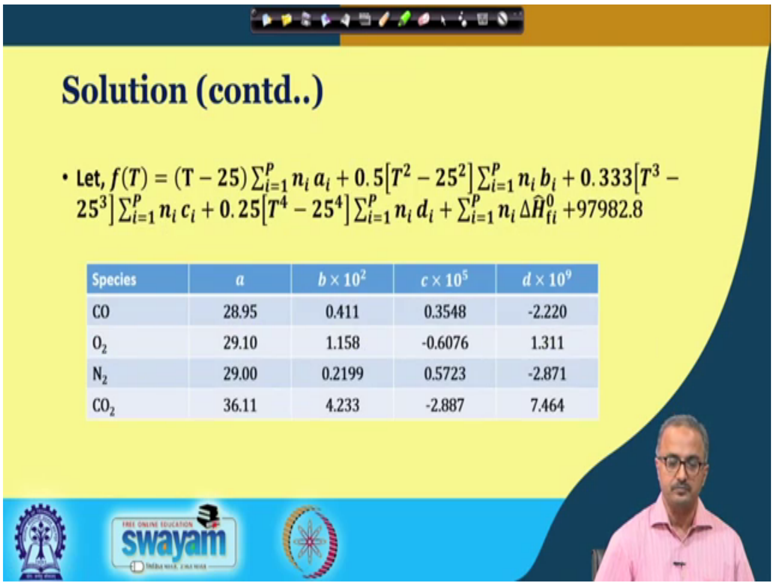

And so, we are basically, we are trying to solve an equation that is the function of temperature and here we put the values of a b c d.

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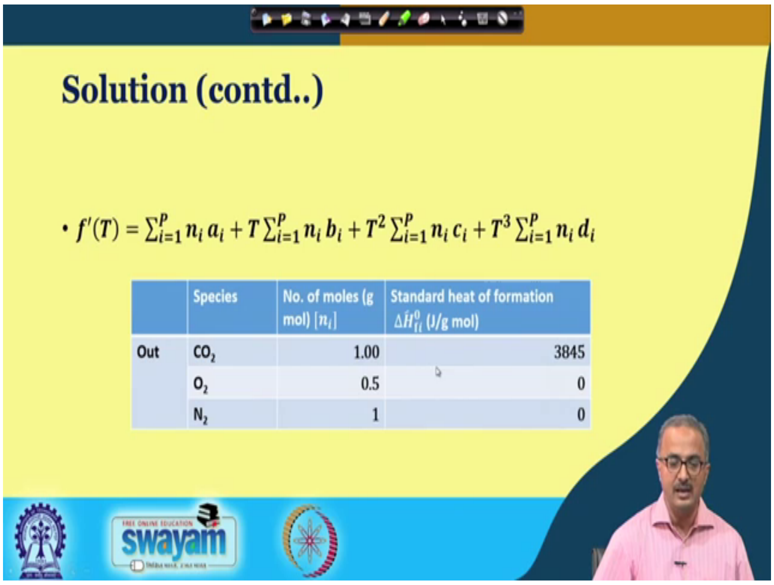

And now, we find that we are using a Newton Raphson Method. So, we have this derivative of the function. Newton Raphson Method, I shall be teaching you in my subsequent lecture, this is one of the ways of finding the root of the non-linear algebraic equations.

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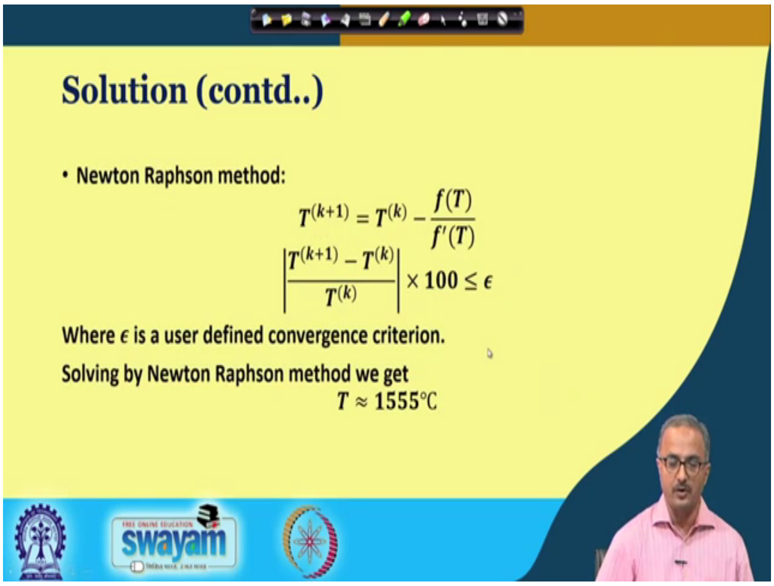

So, we are putting this derivative of the Newton Raphson Method and here we are putting the number of moles and standard heat of formation of all the components. And here this is the recurring formula, recurrence formula in the Newton Raphson Method; that means, in this method what we do that we take some assumed value and keep on updating the value in terms of the function value and the derivative of the function. So, I am not going to details of this particular method, I shall be taking them up later.

So, if the suffice to say is this that here is we put some kind of convergence criterion and this K represents the number of iteration. So, basically we are checking the values in the two consecutive iterations just a, small modification. Here will be that these Ts are calculated at the k th temperature; so, at the kth iteration level, ok. So, it is as, as you can see this is for kth iteration level at the same temperature, we will be calculating this the function value and the derivative of the function.

And then for checking the convergence the user puts some kind of convergence criterion, it could be 1 percent, 10 percent or 0.1 percent depending on the accuracy needed. So, we put that criterion here and then we get some convergence and if you solve this equation, you will find the approximate value of the theoretical flame temperature or adiabatic flame temperature is going to be this value, ok.

So, this is a pretty simple way of putting this, applying the energy balance, because in the energy balance we are assuming the change in the kinetic energy, potential energy to be 0, the adiabatic means Q to be 0 and there is no work done, because a reactor is a fixed reactor rigid reactor, ok. So, when in the energy balance equation when we drop all those terms, we will find that we are having the, the terms which were shown in this particular solution.

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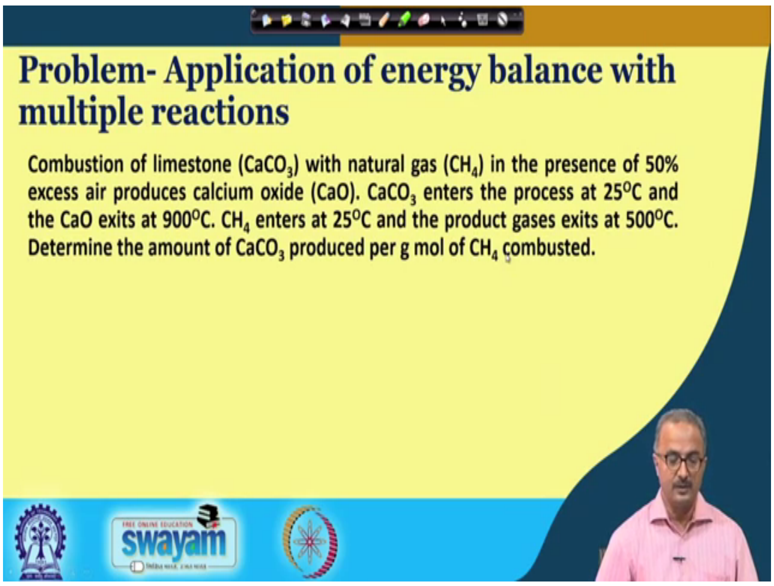

Now, we go to the next problem. In this problem, we are applying the same energy balance equation, but for multiple reactions so far we have looked into one reactions. Now, we are going for multiple reactions, in this we have the combustion of limestone, limestone is calcium carbonate with natural gas that is methane, primarily; in the presence of 50 percent excess air produces carbon calcium oxide that is Ca O and calcium carbonate enters the process at 25 degree centigrade and calcium oxides exits at 900 degree centigrade. Methane enters at 25 degree centigrade and the product gases exit 500 degree centigrade. So, we have to determine the amount of calcium carbonate produced per gram mole of methane combusted, ok.

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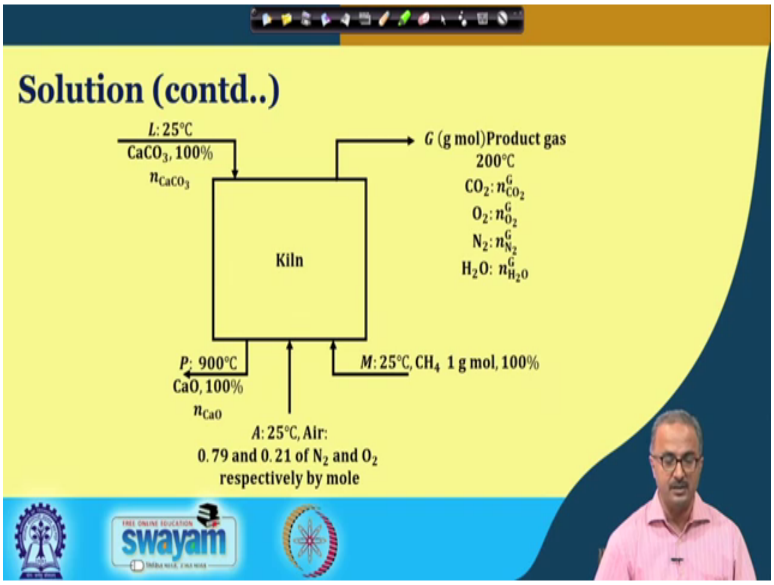

So, with this problem statement now, we show you schematically how this thing looks like. So, here we have the incoming stream of calcium carbonate, ok. This is a kind of kiln in which this reaction is going on and here we have written the conditions of the calcium carbonate as given in the problem. And here, we show it 100 percent that is it is taken to be pure calcium carbonate. And this is the number of moles of calcium carbonate and the another in that stream is the methane here. And all the conditions for the methane are also given here, it is pure methane the natural gas, it is primarily methane, but here we are assuming that it is pure methane stream.

And when we have shown the product streams over here, we are showing this thing on this left hand side, because calcium carbonate is solid so, by gravity it will come down.

And similarly, this calcium oxide is also solid so, it is will be taken from the bottom of the kiln. On the other hand any kind of gases will move up due to buoyancy and they will be collected from the top of the particular reactor, ok. So, they have been shown on the top, ok. And similarly, these gaseous inlet stream is also shown from the bottom, because it will tend to move up the column.

Now, along with methane, we are also sending the air and again we are assuming the air to be a binary mixture of nitrogen oxygen and nitrogen is taken to be 0.79 mole fraction and oxygen taken to be 0.21 mole fraction.

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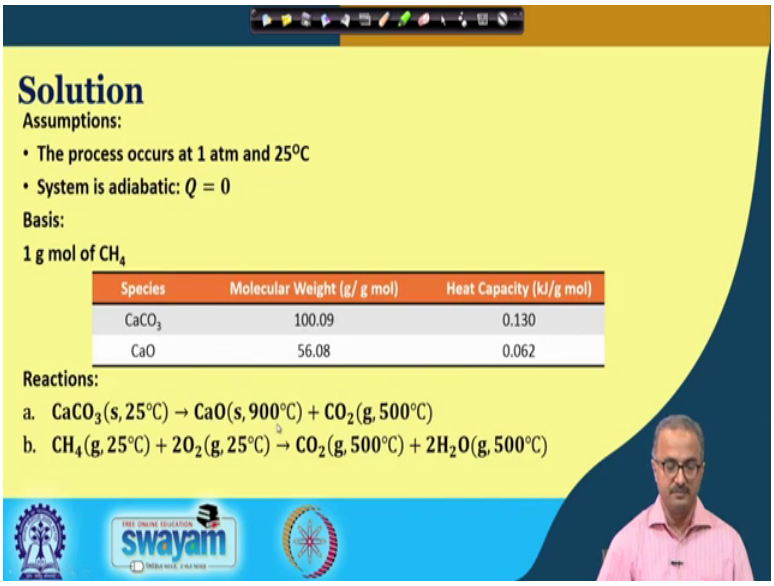

Now, the assumptions are the process occurs at 1 atmosphere and 25 degree centigrade system is adiabatic to Q is 0 and neglecting other terms like changing in kinetic energy, change in the potential energy and there is no work done. So, we shall be arriving at the total change in the process will be simply the change in the enthalpy of the product stream and minus the change in the enthalpy of the raw materials.

So, taking the basis as this 1 gram mole of methane, we write for the species the molecular weight, the heat capacity taken from the literature. And these are the two reactions; one in the first reaction, we find that calcium carbonate is going into to decompose into calcium oxide and carbon dioxide. And in the second reaction what we are finding that methane is combusting with oxygen to give carbon dioxide and water and these are at 5 degrees 500 degree centigrade and this calcium oxide is at 900 degree centigrade.

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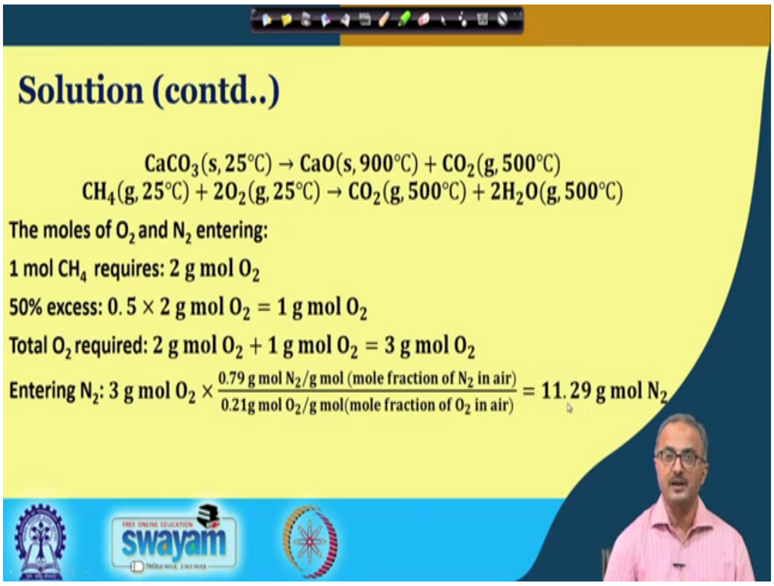

And here you see that with this kind of balances, we have also put the number of moles of oxygen and nitrogen entering the system. So, 1 mole of methane requires 2 gram mole of oxygen as you can find from this stoichiometric equation.

And again we have been told that we are sending 50 percent excess air excess; that means, that 2 gram is needed. And we are putting excess of this that is 1 gram mole is excess and that is total amount of oxygen going into the system is 3 gram mole, ok. And once, we know the amount of oxygen going so, we can find out the how much nitrogen is going into the system. And we can find out the gram mole of nitrogen going inside the system.

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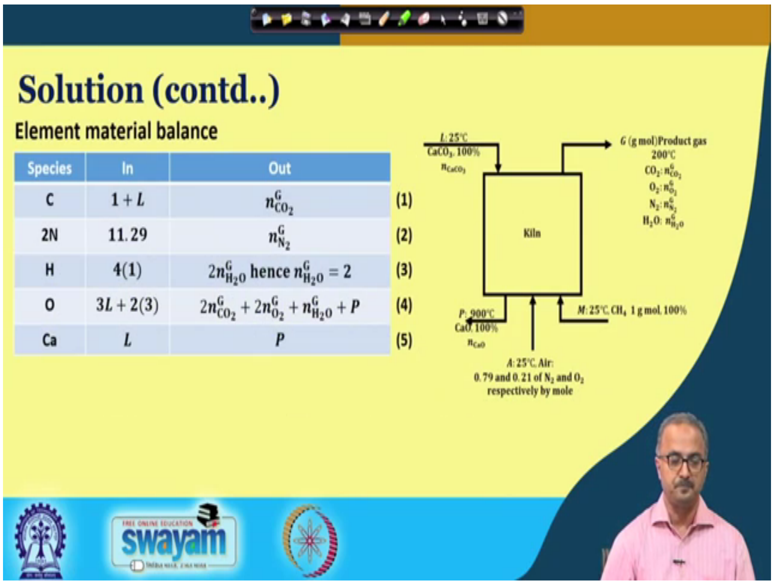

Now, we write the species material balance to find out the number of moles of each of the species. So, here I have shown you for the inlet stream for all each of the individual species over here, ok. And here I have shown you for all the outgoing streams here. So, here I am doing the elemental balance as I told you that in this case elemental balance will be bitter, because we are just trying to find out that carbon is going inside the system. Now, how much carbon is going out of the system and we are not going to go for the delta H reaction that is the heat of reaction.

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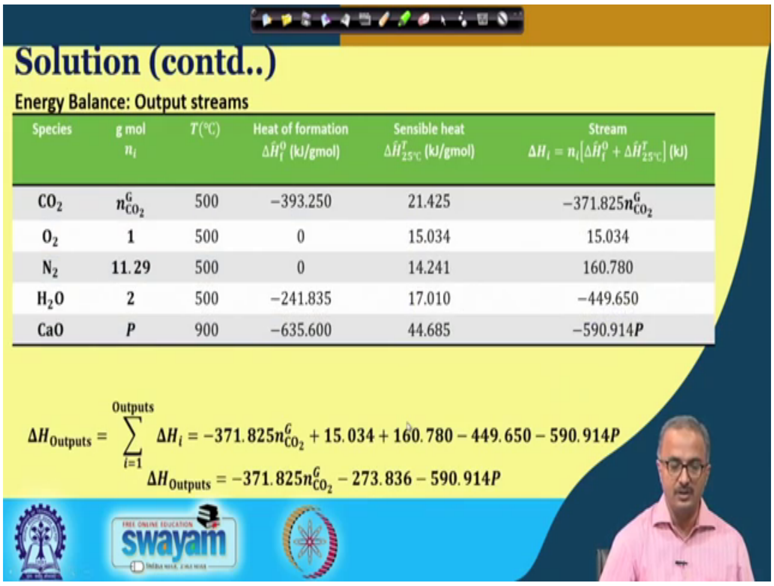

So, we are going with the elemental balance. So, after this what we are doing that we put all these values from the literature heat of formation sensible heat; as sensible heat as you know that we have found it out by the integration of the CP DT. And this is the total heat or change for the all those streams for the output streams and these are pretty straightforward. And since I have explained these things to in the earlier problem so, I am not going into details of this. Once you know the temperatures of the various streams, you can find this particular values very easily by integrating from 25 degree centigrade to these temperatures. And then afterwards you are just simply adding these two and multiplying with the number of moles and now you get this kind of output things.

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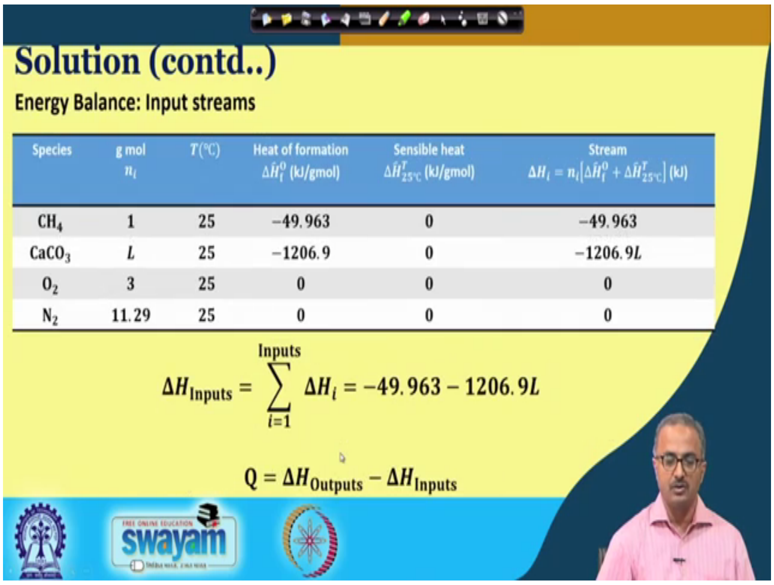

Now, here you see that once you put for the input and output then you find that there are many of these things are unknown, ok. So, you have to know the number of moles of carbon dioxide, you have to know the feed stream velocities. So, what we have whatever equations, we have written earlier. And what we are just rearranging the equations to get the solution for each of the unknown variables. And this is very straightforward basically, you are solving a few coupled linear algebraic equations, ok.

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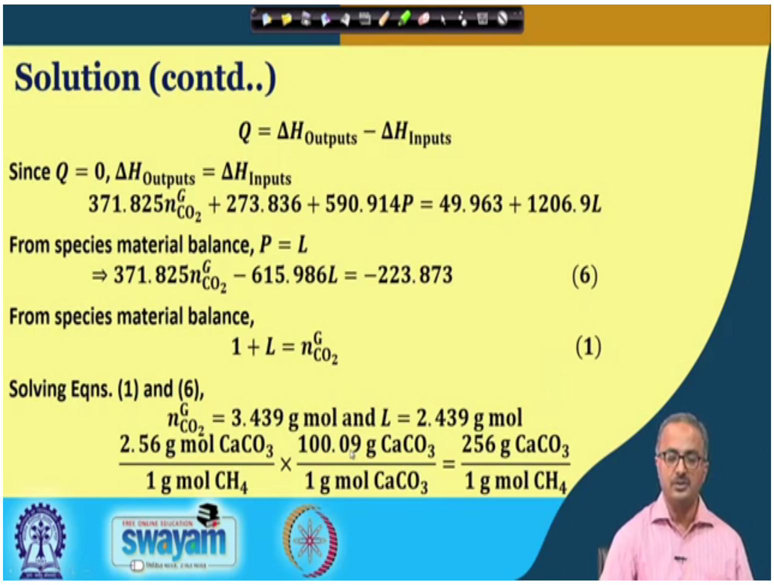

So, I am not going into detail of this solution slso; you can do it very easily and ultimately you find that you are getting these two values. Once you get these two values, now you can find out that how much calcium carbonate is being consumed per unit gram mole of methane by this particular formula, ok. So, this is very straightforward problem.

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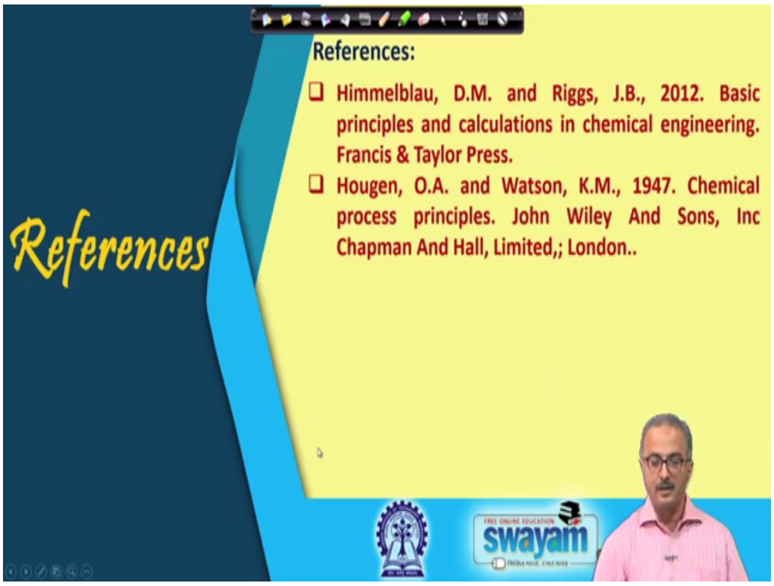

So, more details you can find out from these two books.

Thank you