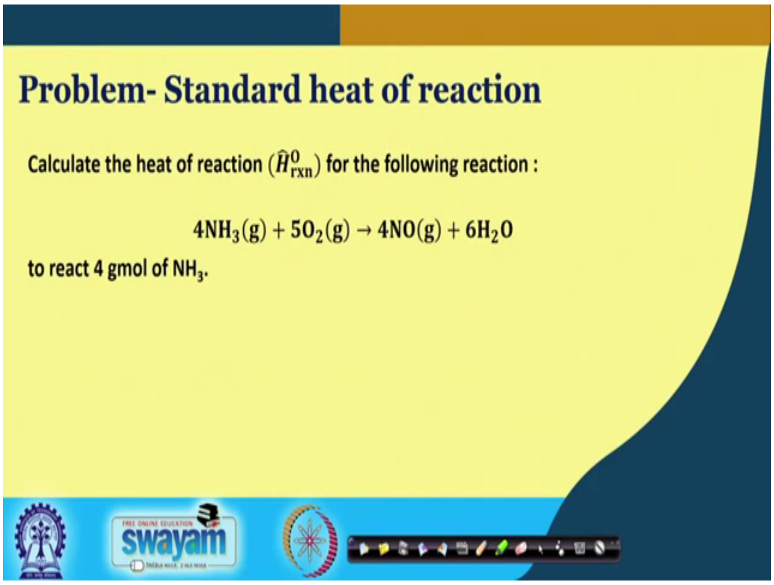
Mass, Momentum and Energy Balances in Engineering Analysis
Prof. Pavitra Sandilya
Department of Cryogenics Engineering Center
Indian Institute of Technology, Kharagpur

Lecture - 14
Energy Interactions in Reacting Systems

Welcome. So far we have seen how the various types of reactions come into the material balance. Now, what we shall do that we will go to the energy balance, before that we and look into the effects of the reaction terms. So, before that what we shall see in this particular lecture is that how we account for the various kind of energy interactions in a reacting system.

(Refer Slide Time: 00:49)

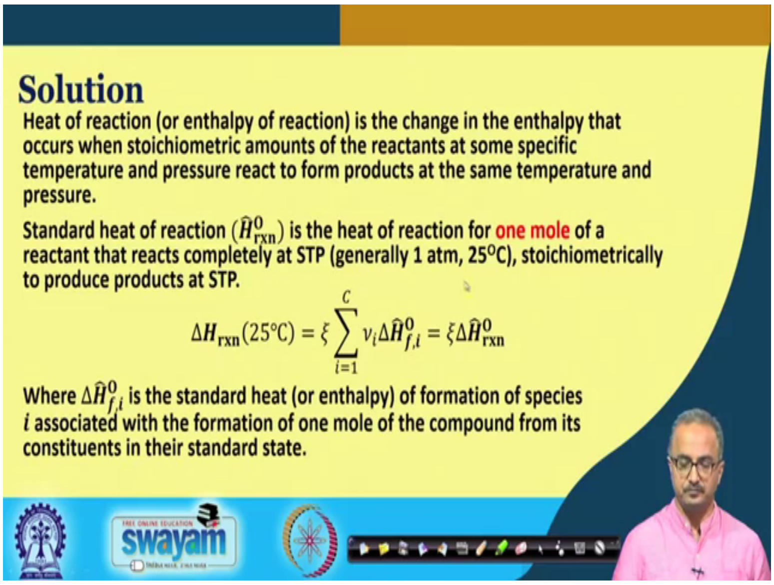


So, first we will demonstrate all these things through some problems. So, we go to the first problem. And in this problem we are required to find out the standard heat of reaction. Please note that there are various types of enthalpies or heat associated with different types of reactions. These reactions could be some chemical reactions, there could be combustion of some fuel which involves the reaction of oxygen with the particular fuel. So, all these things are coming under some reaction and not only this we also have the enthalpy of formation that is the heat energy that liberated or consumed during the formation of some compound.

For example, if you are making carbon dioxide from carbon and oxygen, when this two types of molecules combine, then whatever heat effects are there that is also comes under this heat of reaction. So, all these kind of processes are clubbed together under the heat of reaction. And whenever we are talking of any kind of reactor system or reacting system, in that which have to account for any kind of energy exchanges associated with these processes.

So, in this first we shall do the heat of reaction. And the reaction given is the ammonia reacting with oxygen to give us nitric oxide and water. And please note here that the amount this is a stoichiometric equation. And so we have to find the heat of reaction when 4 gram mole of ammonia reacts.

(Refer Slide Time: 02:35)



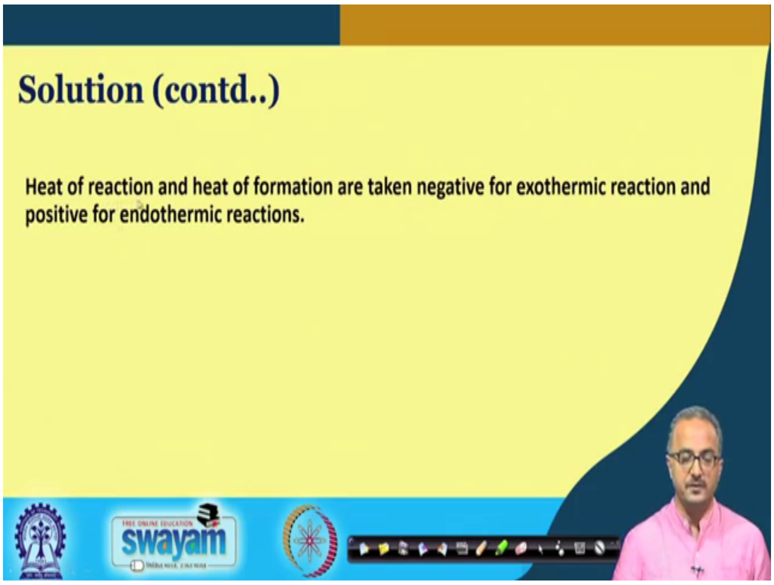
So, first let us see what we understand by heat of reaction, sometimes it is also called enthalpy of reaction. And this is the change in the enthalpy that accompanies the stoichiometric amounts of reactants at some specific temperature, pressure react to form products at the same temperature pressure. That means, whenever there is some kind of reaction going on in stoichiometric amount ok, not in non stoichiometric amount, stoichiometric amount.

So, if the reactants at some given temperature, pressure are forming the products at the same temperature pressure ok. Now, this is very important for us to note that in general whenever some reaction takes place, there could be changes in both the temperature and the pressure ok. However, when we are reporting the heat of reaction, we have to see that all the temperature pressure conditions for both the product and the reactants are the same, so that would need some kind of mathematical manipulation in calculation of the energies associated to do this kind of estimation which we shall see a bit later. So, as of now this is the way we are defining the heat or enthalpy of reaction.

Now, we also have standard heat of reaction which we put in terms like this that H this cap O r x n, r x n stands for reaction. This particular O stands for standard and this cap for per mole per unit mole ok. This is the heat of reaction for one mole of a reactant that reacts completely at STP. STP could be 1 atmosphere, 25 degree centigrade, because this STP may be varying for in you will find in different literature, this STP values may be varying.

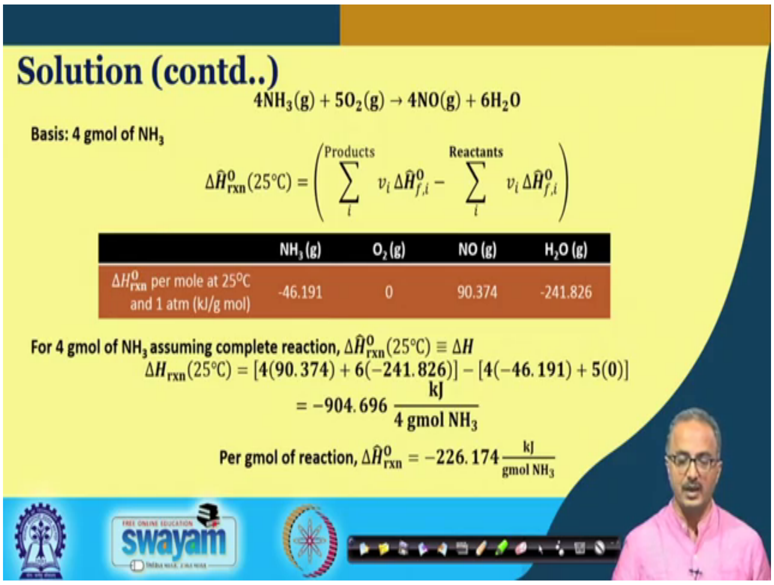
So, what we are saying that 1 mole of the reactant reacts completely at STP stoichiometrically to produce products at STP. So, here we have this that we are not going into the derivation of this particular equation. So, this is suffice to know that here we have the heat of reaction at 25 degree centigrade. And this is given in terms of the heat of formation of the products as well as the reactance. Now, you see depending on the sign of this particular nu that is the stoichiometric coefficient, we are able to account for both the product and the reactants. Here C represents the total number of species in the particular system; the number of species consists both of the reactants and the products. And ultimately we get this particular relationship between the heat of reaction and the standard heat of reaction.

(Refer Slide Time: 05:49)



Now, this heat of reaction and heat of formation are taken negative for exothermic reaction and positive for endothermic reactions by convention. Generally this is the convention, but in the literature you may find the opposite convention may also be used. Now, you perhaps know exothermic reactions are those reactions which involve the liberation of heat on during the product formation. On the other hand endothermic reactions are those reactions when the product formation is accompanied by an absorption of heat. And that we can feel very easily that in case of exothermic reactions the particular vessel will get hotter and in case of endothermic reactions the particular vessel will get cooler.

(Refer Slide Time: 06:41)

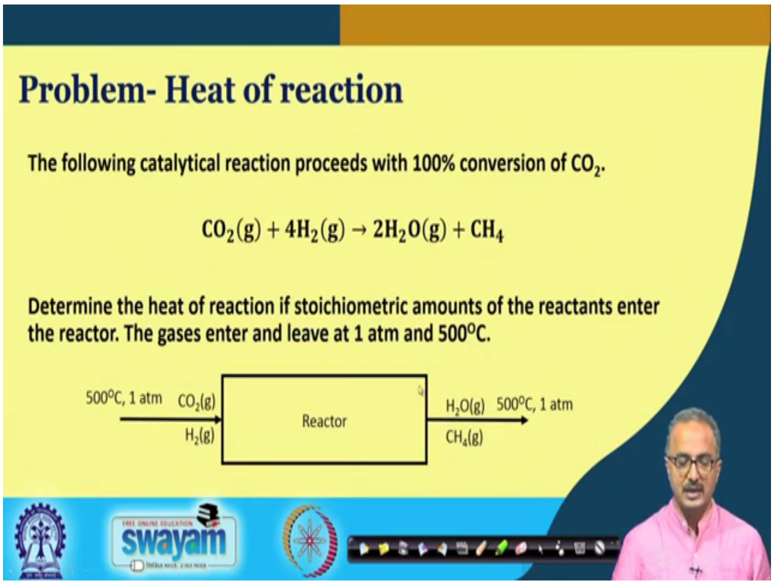


Now, coming back to our problem, let us look at this particular equation. And now we are writing from the definition of the standard heat of reaction this particular formula. Now, you see that all these values of the heat of formation will be given in some standard table. And I have given you the references at the end of this lecture, where which you can refer to get these values of the heat of formation. And you can see that for the pure components only oxygen, there is no heat of formation. For the other compounds we have the heat of formation.

And now once we get this heat of formation values we can plug in their respective stoichiometric coefficients for the product we are putting like here. We have for the NO, this is 4 so, we are putting 4 here. And the heat of formation of NO is 90.374 which we are putting here and for water, it is 6 here, so we are putting 6. And this is the value we are putting over here minus we are going to minus because we are talking about the reactant side so minus 4 for this ammonia and the value of this heat of formation of ammonia and 0 for oxygen.

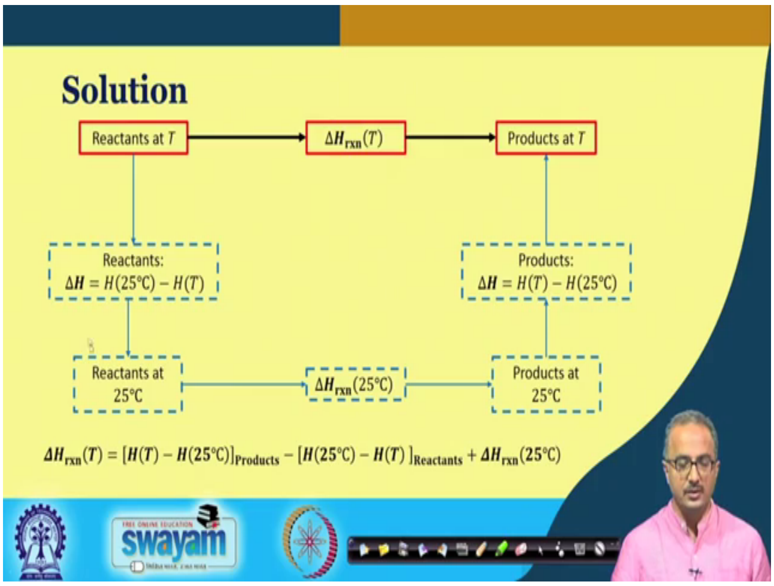
And then after all doing all these things you get this is value of the heat of reaction. And this is for 4 gram mole of ammonia, when 4 gram mole of ammonia are reacting. Now, for mole gram mole of ammonia, we simply divide this value by 4 and we get this value. So, it is quite simple and it is just a manipulation of the heat of formation and the stoichiometric coefficient to get the heat of reaction.

(Refer Slide Time: 08:31)



Next problem is another one for heat of reaction for another kind of reaction that is carbon dioxide is reacting with hydrogen to give H 2 O and methane. So, here we have the system and here we are told that gas enters at 1 atmosphere pressure and 500 degree centigrade temperature it reacts and it gives out the products water vapour and the methane gas at the same temperature as the inlet and same pressure as the inlet ok. So, we have to find out the heat of reaction if stoichiometric amounts of the reactants enter the reactor, that means we are adhering to the exact amount required by the stoichiometry for each of the reactants.

(Refer Slide Time: 09:19)



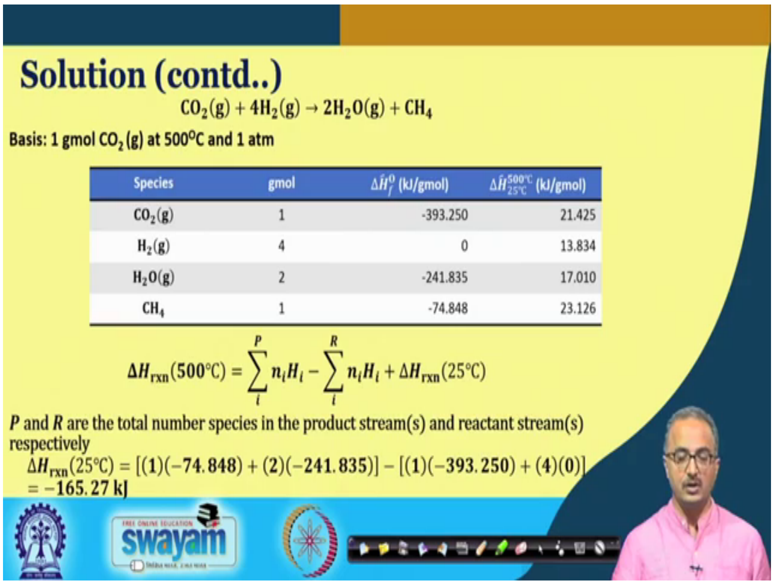
Now, in this particular problem, we see that the temperatures are not the standard temperature. So, this particular line shows that actual case that we have the reactants at some temperature and the heat of reaction is generated at that temperature, so that we are getting the products at that particular temperature. However, we are given the values of this heat of reaction etcetera at some standard value.

So, let us see how to convert this standard value into the values of the heat of reaction at the given temperature. So, this is the way. So, this particular blue coloured path shows how we calculate the heat of reaction for the given temperature. So, what we assume that from the 25 degree centigrade reactants are there and we take it to the given temperature and this involves sensible heat ok. Once it goes to that temperature, then we have the heat of reaction at 25 degree centigrade.

So, from this temperature, we bring it down to 25 degree centigrade and then we carry out the reaction at 25 degree centigrade. And we get the products at 25 degree centigrade and the product temperature is now brought back to the given temperature of the reaction that also involves the sensible heat. That means we are taking the two sensible heats into account to bring the reactant as well as the product from their given condition to 25 degree centigrade.

Now, this is after doing this, we see this is the energy we get that. This particular thing shows that how the product is taken from 25 degree centigrade to the given temperature how the reactants are taken from the given temperature to 25 degree centigrade and then we have the reaction heat of reaction at 25 degree centigrade.

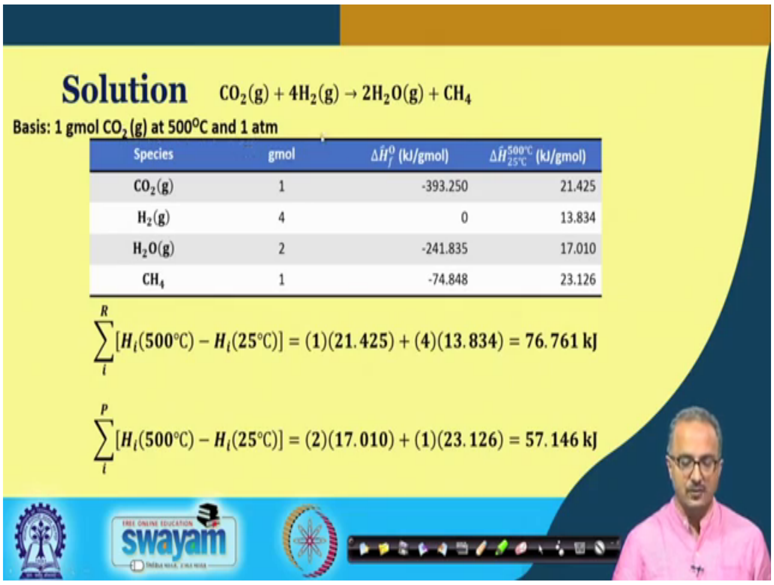
(Refer Slide Time: 11:25)



Now, with that information and the formula, what we shall do, we are now again going back to the problem, we are again getting the values of the heat of formation from the data table. And here we are writing all the stoichiometric gram moles as per the reaction. And here we are putting this particular thing is that we are doing the sensible heat thing which we are putting over here. And you can see that we are writing the heart of reaction at 500 degree centigrade as this is the total the heat that is out the product side this is the total amount of heat that is the reactants side plus the heat of reaction. And here the P and R represent the number of species in the product streams and the reactant streams respectively.

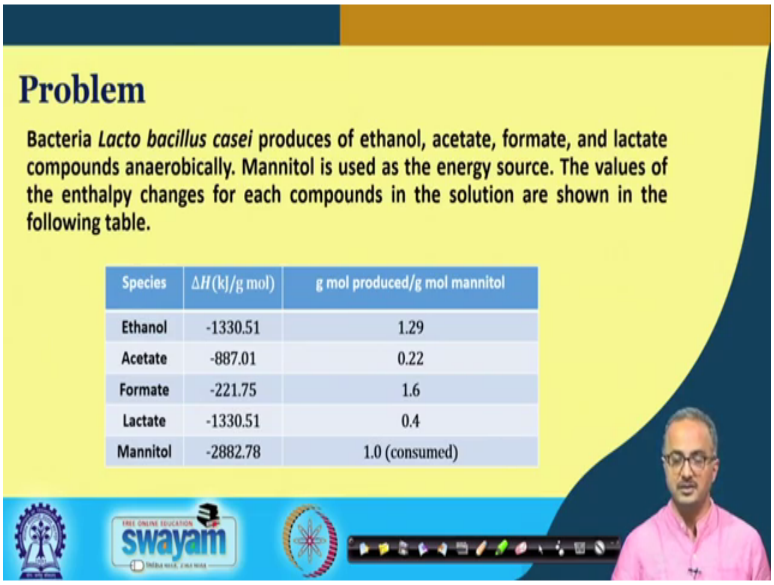
So, here it is simply just we are plugging in the values of this heat of formation over here along with the number of moles which are entering. And in this case is mind because the problems is the number of moles entering the system is same as the stoichiometric amount. So, in this case, we are finding that n i is same as nu i, but in general this n i need not be same as the stoichiometric coefficient, there could be excess of reactants also. In that case, we have to account for the actual number of moles of the reactants ok, so that is why we are putting it ni n naught nu i. So, just plug in the values along with the heat of formation and we are getting this value of the heat of reaction.

(Refer Slide Time: 13:07)



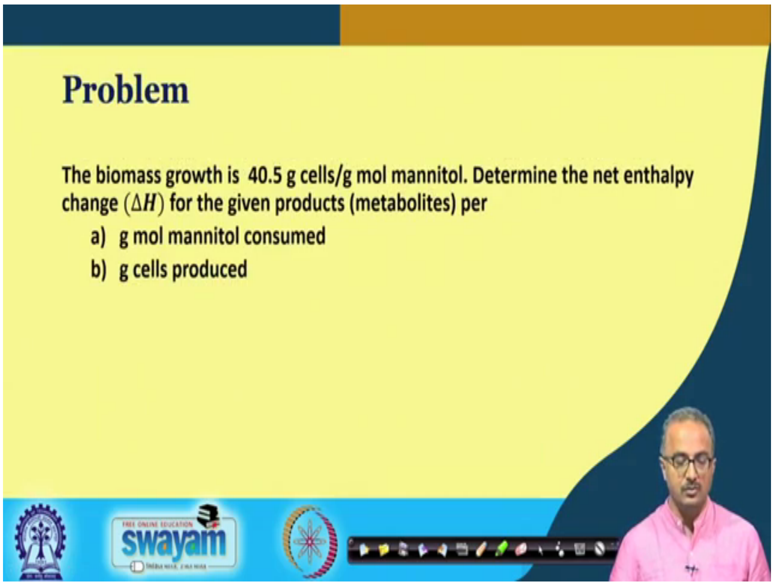
And then we are what we are doing that for this particular thing we are getting this sensible heat terms and this can be also obtained from these values over here. This is basically we are doing the C p dt and for C p o s that is C p means is the specific heat that is specific heat data can also be obtained from the data table from the references I have given at the end of the lecture. You can find the sensible heat terms and ultimately you find the heat of reaction by combining all the terms together. And this is the heat of reaction. And you can see the difference between the standard heat of reaction and the heat of reaction at some other temperature.

(Refer Slide Time: 13:51)



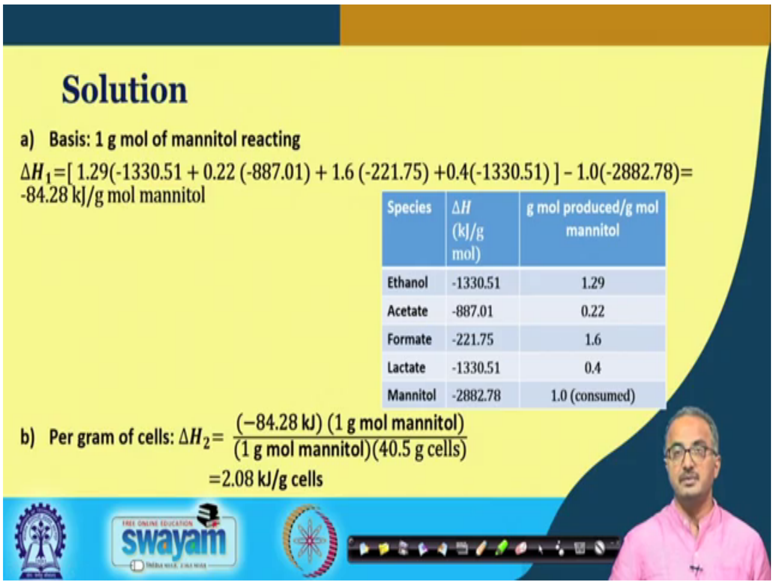
Now, we come to another problem of similar kind. Here we have some kind of bacterial reaction that we know that bacterial reactions are also find in our day-to-day life that. For example, when we are making curd from the milk we know that lacto bacillus bacteria acts on the milk to convert into the curd. So, similar things are also done in the industry for production of many compounds. So, here we have lacto bacillus casei is produces ethanol, acetate, formate, lactate compounds anaerobically that is in the absence of oxygen. And mannitol is used as the energy source. And the values of the enthalpy changes for each compounds in the solution are given in this particular table ok. So, here we have the gram mole produced per gram mole of mannitol for each of these species in the particular system and these are the enthalpy of changes for each of the species ok.

(Refer Slide Time: 14:53)



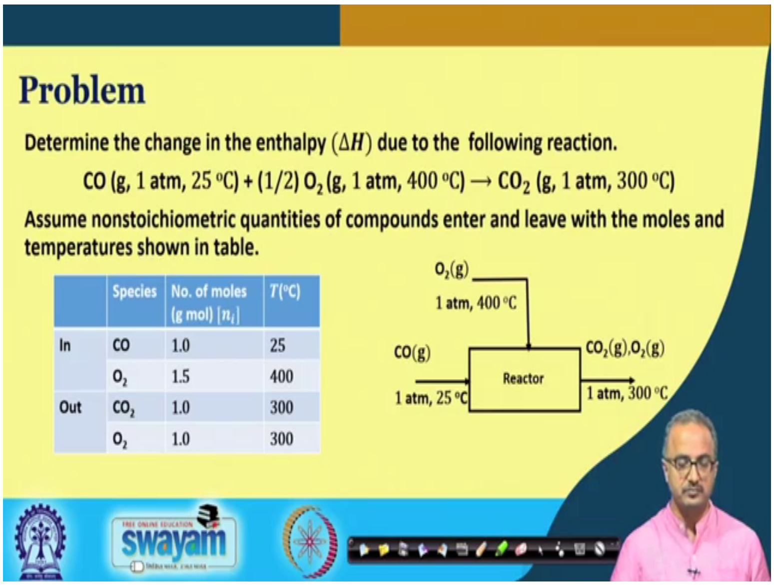
Now, what we have been asked that biomass growth is 40.5 gram cells per gram mole of mannitol. Determine the net enthalpy change for the given products or vardenafil metabolites. Metabolites are the compounds which are produced after some metabolic reaction goes on ok. So, metabolic reactions goes on in any kind of animal body in even in our body, we have many metabolic active activities. So, whatever products are formed, they are called metabolites. So, this particular net enthalpy of change for the given products per gram mole of mannitol consumed and from per gram of cells produced. So, this is what you have to find.

(Refer Slide Time: 15:41)



And it is pretty simple problem. You can see that we just find out the enthalpy change by writing all these respective gram mole along with the enthalpy of formation and we put this here. And now what we do for per gram mole of the cells, what we do that we know that how many cells have been produced per gram mole of mannitol, we put it put this value here. And we get that this is the value of the enthalpy change per gram mole of cells. And this is the value is the enthalpy change per gram of mannitol as obtained from this particular data table. So, this is a pretty straightforward problem.

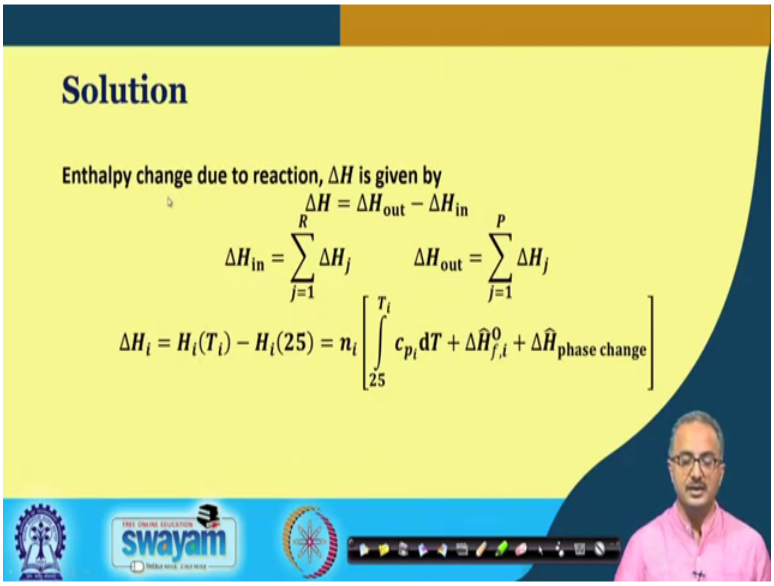
(Refer Slide Time: 16:25)



Next problem we come here that we are finding that in this problem, we are producing carbon dioxide from carbon monoxide. And here these are the temperatures given that the carbon monoxide intercept 1 atmosphere 25 degree centigrade, oxygen enters at 1 atmosphere and 400 degree centigrade. And carbon dioxide and oxygen comes out at 300 degree centigrade and 1 atmosphere. So, you can see there are some unreacted oxygen also coming out in the product, but there are no carbon monoxide in the product.

Now, what we do that here we write the all the species we have and the number of gram moles which are going in and which are coming out and these are the respective temperatures of the various streams. Now, with this information and assuming that nonstoichiometric quantities of compounds enter and leave with the moles and temperature shown in the table that means, these are on nonstoichiometry. Stoichiometry says for each gram mole of carbon monoxide, we need only 0.5 gram mole of oxygen, but what we are doing we are sending much more than that. So, here you see we are sending much more than that ok. So, this oxygen is in excess ok. So, for 1 mole of carbon monoxide, we need only 0.5 mole of oxygen that will rest 1 mole is remaining unreacted and it will get out in the product stream.

(Refer Slide Time: 18:03)

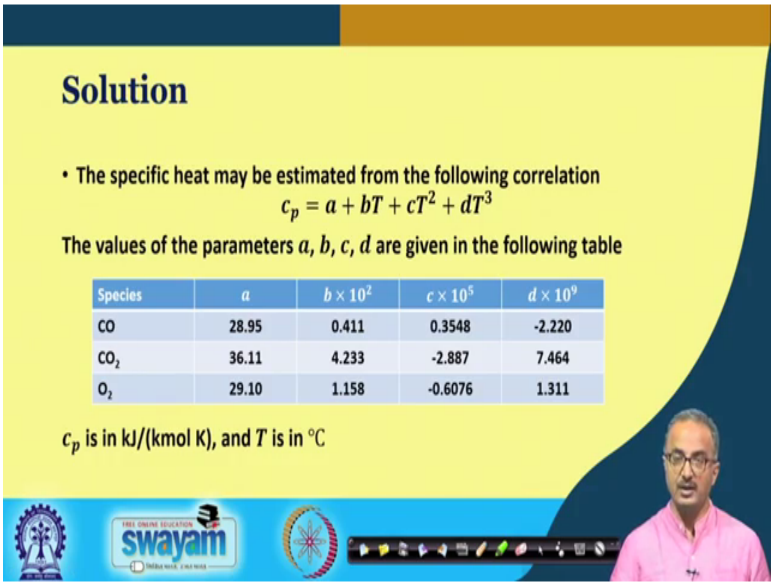


So, you can see here that net enthalpy change of the reaction is given by the change in the enthalpy out and this for the reactant side ok. So, for the total enthalpy change in the input is for all each of the species whatever enthalpy changes are there, we just sum it up.

And for the outgoing streams we sum it up all the enthalpy changes associated with each of the products species ok. And we know that this is the delta H i which has the enthalpy at the given temperature minus the enthalpy at the standard temperature, in this case that is 25 degree centigrade. I am not writing this degree centigrade every time; by default we are assuming that all the temperatures here are in degree centigrade.

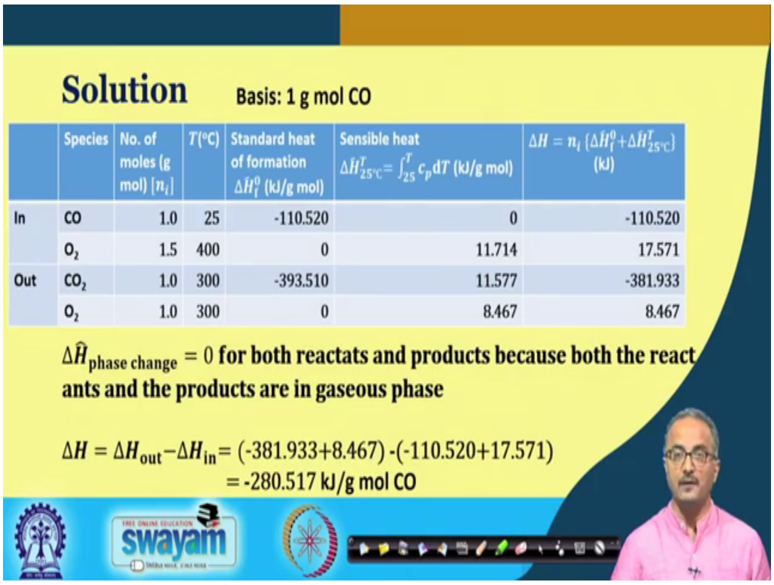
Now, this particular thing is given by this particular equation. And you can see that in this case there could be phase changes also. Suppose the reaction is happening in gaseous phase, but product is coming out in the liquid phase or the reaction is in the liquid phase, the product is coming in the gaseous phase. So, there will be some kind of phase changes also involved ok. But in this particular example, there is no phase change. So, enthalpy change due to phase change will be taken as 0 and rest of the things we shall be accounting for.

(Refer Slide Time: 19:29)



So, again we see that the specific heat may be estimated for various types of correlations. And in the data source, we find that the specific heat for the given components have been given in terms of this polynomial equation. And in this a, b, c, d are specific for a given component. And in this table, I have shown you the values of a, b, c and d and here for this particular values of a, b, c, d the unit of the specific heat is kilojoule per kilo mole Kelvin and the temperature to be taken is in degree centigrade, So, you have to be very careful whenever you are using any kind of correlation about the units ok.

(Refer Slide Time: 20:17)

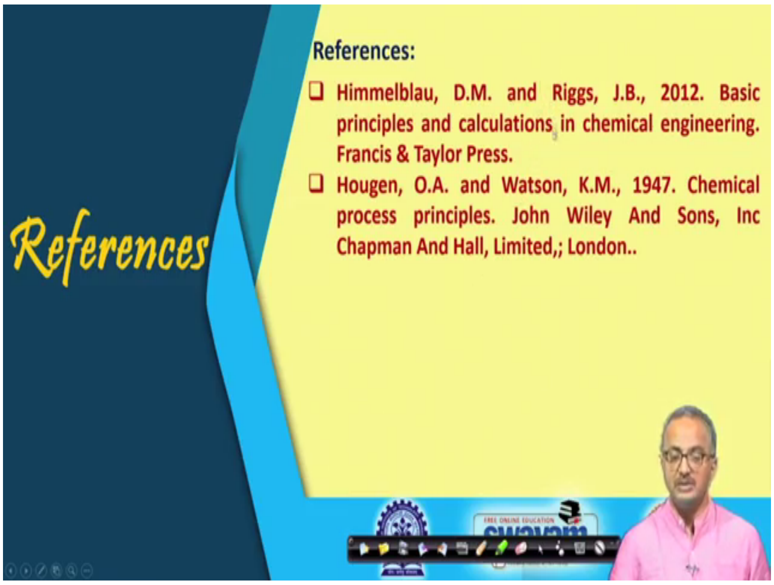


Now, after that what we do that again we reproduce the table, only thing is this we now put some extra values which we need to find out the enthalpy change. First we get the values of the enthalpy of formation from the data table ok. Next is this we get the values of the a, b, c, d as we have just shown you. And now we perform this particular integration to find out the sensible heat contribution ok.

Now, we do this integration and we put the values of this integration values. This you can perform very easily. And then we find out we simply add this value with this value for each of the components over here, only thing is this now this we first we sum these two values and then we multiply with the number of moles, so that we get total change ok, because each of these values are giving for per unit mole. So, we multiplied by the total number of moles to get the total change. So, after we see that this values also may be getting modified especially for oxygen we find that this value is getting modified to this value for rest of the components we find the values are remaining unchanged, because the number of moles for them is 1.

Now, in this case as I told you the change in enthalpy due phase change is taken to be 0 because both the reactants and the products are in the gaseous phase. And now after obtaining this total enthalpy change associated with the reactance and the product, what we simply do, we first sum up the total enthalpy change on the product side and then from that we subtract the total enthalpy change due to the reactants. And this is the value we get for the total change in the enthalpy for one gram mole of CO. Now, please mind the basis over here has been taken to be 1 gram mole of CO as per the question. But, if we change the basis, if or for other thing we want to know the basis, then definitely these values will also be changed ok.

(Refer Slide Time: 22:41)



Now, as I told you these are the two references you can refer to for more information on these concepts plus some more data which I have shown in the problems.

Thank you.