

**Material and Energy Balances**  
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**Lecture - 58**  
**Energy Balances on Reactive Processes - Part 1**

Welcome to today's lecture on energy balances on reactive processes. In the last lecture we looked at the fundamentals associated with reaction process. We have performed enough tutorial problems. We have now established enough understanding of how we can account for reactions while we perform energy balances. Now we will try to apply these fundamentals and try to solve problems where energy balances have to be performed for reactive systems.

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## General Procedures

- Draw and label a flowchart
- Use material balances to determine as many stream component amounts or flow rates as possible
- Choose reference states for specific enthalpy or internal energy calculations
- Prepare an inlet-outlet enthalpy or internal energy table
- Calculate  $\Delta\dot{H}$  (or  $\Delta U$  or  $\Delta H$ )
- Substitute the value in the appropriate energy balance equation
- Complete the required calculations

So we will first start with the general procedure. So this would be very similar to the procedures which we have been doing except that we will now add a few terms to the final equations which we use for change in enthalpy or try to identify different reference states which would help us account for the heat of reaction along with the changes in temperature and phase while we perform energy balances.

So the first step for the general procedure would be to draw and label the flowchart and then you would have to perform all the material balance calculations to obtain as many stream component

amounts and flow rates as possible. So we will perform all material balances. As I have already said, the first step for any energy balance problem is to perform material balances.

So once we complete the material balances, we would have all the information about the flow sheet and once we have the completed flow sheet for the given flow diagram we can start with the energy balance aspect. So first step would be to identify appropriate reference states for the different components which are present in the system. So we will have to identify these reference states for every different chemical component present in the system.

So we will have to identify what phase, temperature and pressure these components will be present in and identify them as the reference states while we build the enthalpy or the internal energy tables. Then you will prepare the inlet and outlet enthalpy table or the internal energy table so where we will try to identify which terms will go to 0 and which would be nonzero terms.

And then we will be calculating the total change in specific enthalpy or the total change in specific internal energy and finally convert them into change in total enthalpy and total internal energy and these values will be used in the general energy balance equation for the open or close system to perform the energy balance to get the parameters which we are looking for. So the procedure itself is quite similar to whatever we have been doing till now.

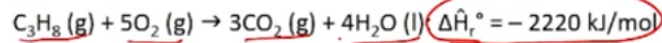
Only difference is the step where we identify the reference states. So it all depends on what reference states we are going to identify. So if we are going to identify an appropriate reference state then we would have to use the heat of reaction which we either get from the problem statement or we calculate using Hess's law and use this heat of reaction in the equation where we calculate the total change in enthalpy.

If we choose a different set of reference states then we can actually intrinsically account for the heat of reaction. We will look at how we can do that. We will talk about the two techniques which can actually enable us to do either of them. So once we finally do all this, we will be completing all the required calculations to obtain the parameters which we are looking for.

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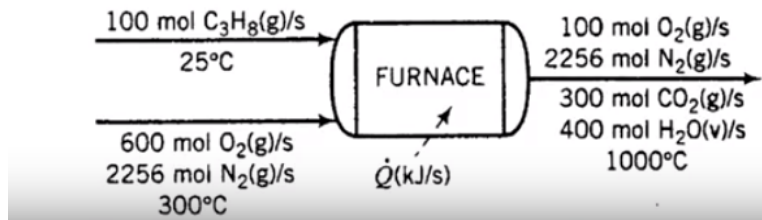
## Example #1

- Propane is burned in the furnace. The combustion reaction that occurs is:



Calculate the rate of heat transfer for the following process using

- Heat of reaction method ✓
- Heat of formation method



So here is an example problem where we have been asked to perform energy balances for a reactive system. Propane is burned in the furnace. Combustion reaction which occurs is propane gas reacts with oxygen gas to form carbon dioxide gas and water liquid and for this reaction you have the heat of reaction which is given as -2220 kJ/mol. You are asked to calculate the rate of heat transfer for the following process using heat of reaction method and heat of formation method and the flowchart gives all the details.

You have 100 moles of propane gas entering at 25 degree Celsius per second and you have air which is a mixture of oxygen and nitrogen and the composition of oxygen and nitrogen in this mixture is also given and this is entering at 300 degree Celsius and so which is basically 600 moles of oxygen per second and 2256 moles of nitrogen per second entering at 300 degree Celsius and you have the exit stream which contains 100 moles of unreacted oxygen which is leaving and 2256 moles of nitrogen which is leaving per second.

You also have 300 moles of carbon dioxide and 400 moles of water vapor which are leaving per second. So this exit gas which is the gas which is produced after combustion, these combustion gases are leaving at a temperature of 1000 degree Celsius. So now the question is to identify at what rate heat must be transferred for the following process. And we have been asked to identify this value for  $Q$  using two techniques.

One is the heat of reaction method and the other is the heat of formation method. What are these? So heat of reaction method is the method which is preferred when you have a single reaction and you have the heat of reaction listed. So you would have the value given and basically you would use this while you calculate the total change in enthalpy. So this is called the heat of reaction method. And heat of formation method is the method where you would be using heat of formation while you are building the internal energy or enthalpy tables.

So basically between these two the fundamental difference is the reference state which is chosen. So the first method is the heat of reaction method where you would actually be using the reference states which are there in the reaction. So you use propane gas, oxygen gas, carbon dioxide gas and water liquid at 25 degree Celsius which is where the standard heat of reaction would be calculated and if you use this as the reference state you can use the heat of reaction which has been given to you in the problem directly while you are calculating the total change in enthalpy. So that would be the heat of reaction method.

So this method is preferred when you have a single reaction where the heat of reaction is more. The second method is the heat of formation method. Here you would inherently use the heat of reaction instead of explicitly using it. So how you do that is you use the reference states which would be used for the formation reaction. So we already know what formation reaction is. So basically elements which exist in its native form have to come together to form a compound.

So for example in this case you would use carbon solid, oxygen gas and hydrogen gas as the reference states and if you were to use that as the reference states then you would be using, you would be building the enthalpy table which would account for the heat of formation as part of the step where from the reference state of carbon and oxygen it goes to carbon dioxide and then the next step would be where you have the heating.

So with this kind of a process you would account for the heat of reaction in an implicit way. So the idea is to try and do this together. So we will see how this actually works and we will try to solve the same problem using both the techniques. So obviously you would end up with the same

values but we want to learn both the techniques and get familiarized with these concepts. So once we do that we would also look at how heat of formation method actually implicitly accounts for the heat of reaction while you perform the calculations, okay? Let us start with this problem.

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Example #1

$$Q - \dot{W}_s = \Delta \dot{H} + \Delta \dot{E}_k + \Delta \dot{E}_p$$

$$Q = \Delta \dot{H}$$

Ref. state:  $C_3H_8(g), O_2(g), CO_2(g), H_2O(l), N_2(g)$  at 25°C, 1 atm

	$\dot{n}_{in}$	$\hat{H}_{in}$	$\dot{n}_{out}$	$\hat{H}_{out}$
$C_3H_8(g)$	100	0	—	$\hat{H}_4$
$O_2$	600	$\hat{H}_2$	100	$\hat{H}_5$
$N_2$	2256	$\hat{H}_3$	2256	$\hat{H}_5$
$CO_2$	—	—	300	$\hat{H}_6$
$H_2O$	—	—	400	$\hat{H}_7$

So the first step for any energy balance problem is to perform material balances. Here all the flow rates are known. So we do not need to perform any material balances. We can start with the energy balance aspect. So the first step is to identify what type of a system it is, whether it is an open or a close system. You have flow rates coming in and flow rates leaving the system. So it would be an open system.

For an open system, the equation, general energy balance equation is  $Q \dot{-} - W_s \dot{-} = \Delta \dot{H} \dot{+} + \Delta \dot{E}_k \dot{+} + \Delta \dot{E}_p \dot{+}$ . So here you do not have any moving parts. So shaft work goes to 0. There is no kinetic or potential energy changes. So the equation gets simplified to  $Q \dot{+} = \Delta \dot{H} \dot{+}$ . So you need to calculate  $\Delta \dot{H} \dot{+}$  which is what we have been doing till now. So now this  $\Delta \dot{H} \dot{+}$  needs to account for the heat of reaction as well.

So how do we do that? So we are not going to look at the heat of reaction method. So for that we need to identify what would be the reference states which we want to use. So as I said, we want to use the heat of reaction which is given. So we need to use the reference states that have been

used to calculate the heat of reaction itself. The standard heat of reaction which is given would be for the compounds and elements in that particular reaction in that phase at 25 degree Celsius.

So we will use that as the reference state. So the reference states we start with would be propane gas, oxygen gas, carbon dioxide gas and water liquid which are all the components which are taking part in the reaction and you also have nitrogen which is not taking part in the reaction, nitrogen gas. We will take all at 25 degree Celsius and 1 atmosphere which is what the reaction would have, the heat of reaction would have accounted for.

So for this we now need to build the enthalpy table. So let us build the inlet and outlet enthalpy tables. So the substances which we have to account for are propane gas. You have oxygen, you have nitrogen, you have carbon dioxide and water. So you have flow rate in as  $\dot{n}$  and enthalpy, specific enthalpy of inlet stream as  $H_{cap\ in}$ . You have  $\dot{n}$  out and  $H_{cap\ out}$ . So based on the information we have from the flow chart, the inlet flow rate for propane is 100 moles per second. Oxygen is 600 moles per second and nitrogen is 2256 moles per second.

There is no carbon dioxide or water vapor entering into, water entering into the system. Whereas in the outlet stream you have no propane. You have 100 moles of oxygen and you have 2256 moles of nitrogen which is leaving the system. In addition to this, you also have 300 moles of carbon dioxide and 400 moles of water vapor leaving the system. So now let us identify which enthalpies will go to 0.

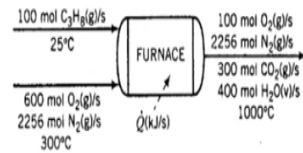
So the specific enthalpy for the inlet propane gas would be 0 because you have propane gas at 25 degree Celsius and 1 atmosphere. So this would be 0 and oxygen and nitrogen are coming in at 300 degree Celsius, our reference state is at 25 degree Celsius. So these would have enthalpy values which have to be calculated. We will call these as  $H_2\ cap$  and  $H_3\ cap$ . So these two components are not present in the inlet stream.

So again, propane is not present in the outlet stream. So these components are all ignored. So we are now left with the outlet stream for which the gases are leaving at 1000 degree Celsius and our reference state is at 25 degree Celsius which means all these streams would have a specific

enthalpy value. So H 4 cap, H 5 cap, H 6 cap and H 7 cap all have to be calculated. Now our goal is to identify the values for all these specific enthalpies.

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### Example #1



$$\hat{H}_2: O_2(25^\circ C) \rightarrow O_2(300^\circ C)$$

$$\hat{H}_2 = 8.47 \text{ kJ/mol}$$

$$\hat{H}_3: N_2(25^\circ C) \rightarrow N_2(300^\circ C)$$

$$\hat{H}_3 = 8.12 \text{ kJ/mol}$$

$$\hat{H}_4: O_2(25^\circ C) \rightarrow O_2(1000^\circ C)$$

$$\hat{H}_4 = 32.47 \text{ kJ/mol}$$

$$\hat{H}_5: N_2(25^\circ C) \rightarrow N_2(1000^\circ C)$$

$$\hat{H}_5 = 30.56 \text{ kJ/mol}$$

$$\hat{H}_6: CO_2(25^\circ C) \rightarrow CO_2(1000^\circ C)$$

$$\hat{H}_6 = 48.6 \text{ kJ/mol}$$

So let us start with H 2 cap. So what is H 2 cap? It is oxygen which is in the reference state of 25 degree Celsius being heated to the inlet condition which is 300 degree Celsius. So H 2 cap is basically oxygen at 25 degree Celsius going to oxygen at 300 degree Celsius. So this value can actually be obtained from the enthalpy table for combustion gases. So it can be obtained from Felder Rousseau in table B.8 and it can be obtained from other textbooks and handbooks as well.

So this will then be H 2 cap = 8.47 kJ/mol. So now similarly we can calculate H 3 cap. H 3 cap would be nitrogen going from 25 degree Celsius to nitrogen at 300 degree Celsius. So your H 3 cap would be equal to 8.12. So this would also be kilo joules per mole. And again this can be obtained from the enthalpy table for combustion gases. So what about H 4 cap? So H 4 cap is oxygen from reference state which is 25 degree Celsius going to oxygen at outlet condition which is 1000 degree Celsius.

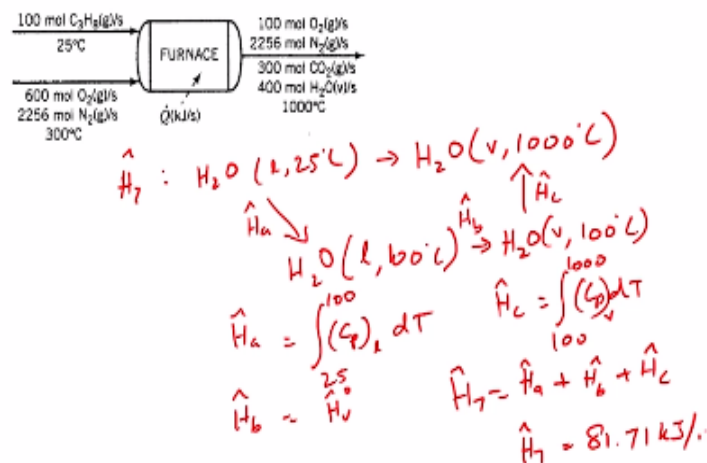
So what you have here H 4 cap which would be equal to 32.47 kJ/mol. Again this value can be obtained from the combustion gas tables for enthalpy and H 5 cap would be similar value for nitrogen. Nitrogen at 25 degree Celsius reference going to nitrogen at 1000 degree Celsius which

is the exit stream. So H 5 cap would be equal to 30.56 kJ/mol. So now you have H 6 and H 7 cap.

So H 6 cap you basically can use the table for combustion gases and you would be able to get the value for carbon dioxide being heated from 25 degree Celsius which is the reference state to carbon dioxide in the exit stream which is 1000 degree Celsius. So your H 6 cap = 48.6 kJ/mol. So now we have H 7 cap which needs to be calculated. What is H 7 cap?

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### Example #1



So H 7 cap here is basically water liquid at 25 degree Celsius going to water vapor at 1000 degree Celsius. So this value needs to be obtained and you could either use steam tables to obtain this value or you would have to use, so basically you would use steam tables to get the value for water liquid at 25 degree Celsius and water vapor for 1000 degree Celsius and find the difference or you could basically perform a calculation where you have a hypothetical path built.

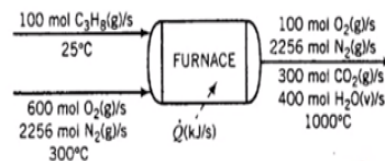
So the hypothetical path would be water goes to water liquid from at 25 degree Celsius goes to water liquid at 100 degree Celsius from where it goes to water vapor at 100 degree Celsius and from here it goes to water vapor at 1000 degree Celsius. So if you were to do this what you would have is so let us say, let us call these as H a cap, H b cap and H c cap. H a cap would be basically integral C p of water liquid dT going from 25 to 100.



H b cap would be equal to the heat of vaporization, standard heat of vaporization for water and H c cap would be equal to integral C p dT where C p is for water vapor from 100 degree Celsius sorry from 100 degree Celsius to 1000 degree Celsius. So your H 7 cap would be equal to H a cap + H b cap + H c cap. So use this or you use the steam tables for the values for enthalpy of water liquid at 25 degree Celsius and water vapor at 1000 degree Celsius and find the difference. Either way, you would end up with H 7 cap as 81.71 kJ/mol.

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## Example #1



$$\dot{\Delta H} = \sum \dot{n}_{out} \hat{H}_{out} - \sum \dot{n}_{in} \hat{H}_{in} + \sum \xi_j \Delta H_{r,j}^{\circ}$$

$$\xi_j = \frac{\text{Moles out} - \text{moles in}}{\nu}$$

$$= \frac{0 - 100}{-1} = 100 \text{ mol}$$

Until now after we get these values, we will plug them back into the specific enthalpy table and basically calculate the total enthalpy of the outlet stream and the total enthalpy of the inlet stream and find the difference to understand what is the total change in enthalpy. However, here in addition to these two differences, you also have to account for the heat of reaction. So how do we account for the heat of reaction?

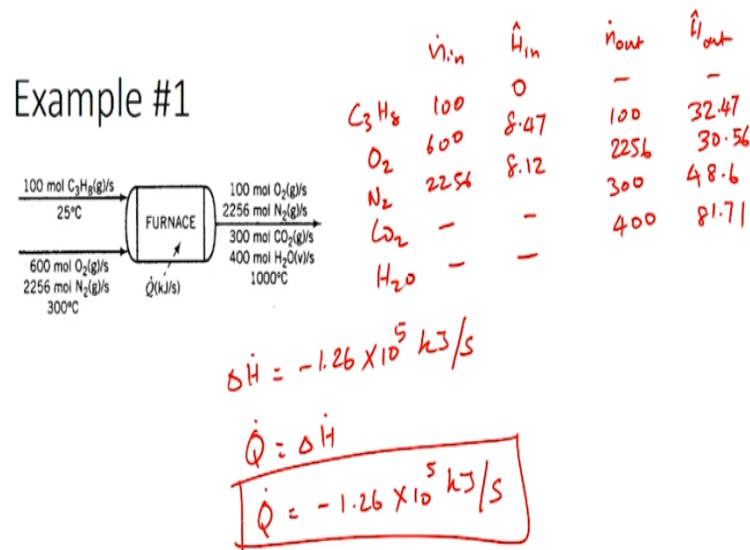
So what we do is the equation delta H dot which was just sigma of n out dot H cap out – sigma of n in dot H in cap. So this was the equation we had been using till now would now have another term which is sigma of psi j delta H r cap j. So this psi stands for the extent of reaction and delta H r basically is the heat of reaction for that particular reaction.

So once we have all the extents of reactions for different equations and the heats of reactions for the different equations, we can multiply the two and we would be able to get the enthalpy change

associated with that particular reaction. So summation of all these values will give you the total change in enthalpy associated with the reactions. So for this we need to know what the extent of reaction for the reaction we have is.

So extent of reaction is calculated as moles out - moles in/ the stoichiometric coefficient. So here let us take propane as the gas as the reactant which is taking part in the reaction. So moles out is 0, moles in is 100 and the stoichiometric coefficient would be negative 1 because it is a reactant with a stoichiometric coefficient of 1. So this would mean the extent of reaction is 100. So 100 moles of the compound is getting reacted with this reaction. So using this extent of reaction we can plug the values back into this equation and calculate the total change in enthalpy.

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So what we would have in the table would be you have propane, oxygen, nitrogen, carbon dioxide and water and the inlet flow rates  $\dot{n}_{in}$  and  $\hat{h}_{in}$ ,  $\dot{n}_{out}$  and  $\hat{h}_{out}$  can all be written down as 100, 600, 2256 and 0 and 0. So this values for the outlet stream would be 100 moles of oxygen, 2256 of nitrogen, 300 moles of carbon dioxide and 400 moles of water.

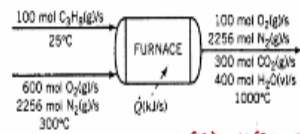
So the enthalpies we have calculated are 0, 8.47, 8.12 and you have 32.47, 30.56, 48.6 and the last one which we calculated was 81.71. So now that we have all these enthalpies we can basically calculate the total enthalpy of the outlet stream as 100 times 32.47 + 2256 times 30.56

+ 300 times 48.6 + 400 times 81.71. Similarly, for the inlet stream it would be 100 times 0 + 600 times 8.47 + 2256 times 8.12.

So the difference between the two can be calculated and you can add that to the extent of reaction times heat of reaction. So your delta H dot is now equal to, so your delta h dot is now = -1.26 times 10 power 5 kJ/s. So substituting this back into the general energy balance equation we had Q dot = delta H dot so which means Q dot = -1.26 times 10 power 5 kJ/s. So this is the value we have for Q. So this way we have actually applied the heat of reaction directly and we have been able to solve the problem.

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### Example #1

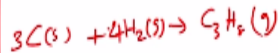


Ref state:  $(C(s), H_2(g), O_2(g), N_2(g))$  at 25°C

	$n_{in}$	$\hat{H}_{in}$	$n_{out}$	$\hat{H}_{out}$
$C_3H_8$	100	$\hat{H}_1$	-	-
$O_2$	600	$\hat{H}_2$	100	$\hat{H}_4$
$N_2$	2256	$\hat{H}_3$	2256	$\hat{H}_5$
$CO_2$	-	-	300	$\hat{H}_6$
$H_2O$	-	-	400	$\hat{H}_7$

$\hat{H}_1: C(s), H_2(g)$  at 25°C

$C_3H_8(g)$  at 25°C



$$\hat{H}_1 = (\Delta \hat{H}_f^0)_{C_3H_8}$$

$$\hat{H}_1 = -103.8 \text{ kJ/mol}$$

$$\hat{H}_2 = 8.47 \text{ kJ/mol}$$

$$\hat{H}_3 = 8.12 \text{ kJ/mol}$$

$$\hat{H}_4 = 32.47 \text{ kJ/mol}$$

$$\hat{H}_5 = 30.56 \text{ kJ/mol}$$

Now let us look at the heat of formation method. So in the heat of formation method, we would prefer to use it when you have multiple reactions or when you have a reaction where the heat of reaction is not readily available. So we will see how a heat of formation method can be used and how it will be different from the heat of reaction. So the fundamental difference as I had already mentioned would be associated with the reference state which is chosen.

So we will look at how to actually use the new reference state and use heat of formation and I will also discuss how heat of formation method implicitly accounts for the heat of reaction and we will look at Hess's law being applied here as a way of accounting for the heat of reaction. Let

us see how this method goes. As usual the first step is to perform material balance calculations. Here there are no material balance calculations required.

So the next step is to identify the type of system and we have already done that and the equation was simplified to  $\dot{Q} = \dot{\Delta H}$ . So let us start with identifying the appropriate reference states. As I had already mentioned, here this is the heat of formation technique. So we need to identify the reference states which would be used in the formation reactions. We want to use the heat of formation of the compounds which means the reference states we choose should be the reference states which are used to measure the standard heat of formation.

So therefore, we would be using the elements as they occur in nature at 25 degree Celsius at 1 atmosphere so that we can account for the heat of formation values. So taking that into consideration, let us now build the enthalpy table with the appropriate reference states. So the reference states would be carbon solid, hydrogen gas, oxygen gas, and nitrogen gas all at 25 degree Celsius and 1 atmosphere.

Because this is the elemental forms which would be used in the heat of formation method. And this would be the reference state where we can actually use the standard heat of formation which can be obtained from tables. Now that we have identified the appropriate reference states, let us start building the specific enthalpy table. So the substances are the same. You have propane, oxygen, nitrogen, carbon dioxide and water. So you have  $n$  in  $\dot{H}_{cap}$  in.

You also have  $n$  out  $\dot{H}_{cap}$  out. So the molar flow rates are the same as what we had done earlier. So it will be 600, 600, 2256 and dash and dash. You do not have any propane leaving the system. You have 100 moles of oxygen, 2256 moles of nitrogen and 300 moles of carbon dioxide and 400 moles of water leaving the system. So here we now need to identify which enthalpies will go to 0. Let us look at which enthalpies can go to 0.

So our reference state is elements in the natural state at 25 degree Celsius, right? So here we have propane entering at 25 degree Celsius. However, our reference state does not include propane. It only includes the carbon and hydrogen. So there would be some change in enthalpy

where the carbon and hydrogen becomes the propane which is the heat of formation. So this would have an enthalpy value which is  $H_1$  cap. Oxygen is coming in at 300 degree Celsius.

Our reference is at 25. So this would be this needs to be calculated as  $H_2$  cap. Similarly, for nitrogen you would have  $H_3$  cap and so on. So you can again write it for the exit streams as well. So you would have  $H_4$  cap,  $H_5$  cap,  $H_6$  cap and  $H_7$  cap. So you now have 7 enthalpy values which we need to calculate. Let us now see what is actually the process where this enthalpy is being formed. So what we have is for let us look at  $H_1$  cap. So what is  $H_1$  cap?

So you have the reference state which is carbon solid and hydrogen gas all at 25 degree Celsius and 1 atmosphere going to  $C_3H_8$  gas at 25 degree Celsius. So this is nothing but the formation reaction where it is carbon solid plus hydrogen gas forming  $C_3H_8$  gas. So if you were to balance the equation, 3 moles of carbon reacts with 4 moles of hydrogen to form 1 mole of propane. So this is the heat of formation which would be the change in enthalpy.

So we can use this and we can get the heat of formation from the tables or textbooks which we have. So the heat of formation for propane gas would be equal to  $H_1$  cap. So  $H_1$  cap =  $\Delta H_f$  degree of propane. So this value can be obtained from any of the tables. So  $H_1$  cap from the tables for heat of formation can be identified as -103.8 kJ/mol. So this would be the value we fill in here. Now we need to identify similar values for  $H_2$  cap,  $H_3$  cap,  $H_4$ ,  $H_5$ ,  $H_6$  and  $H_7$ .

So if you look at  $H_2$ ,  $H_3$ ,  $H_4$  and  $H_5$  you are talking about elements, right? So it is nitrogen and oxygen in their elemental forms. So this is being heated from 25 degree Celsius at reference state to 300 degree Celsius in the inlet condition and 1000 degree Celsius in the outlet condition. So this means these would be processes where you only have change in temperature which was exactly the same as what you had in the previous method which is the heat of reaction method as well. So let us not waste time trying to explain what that process is.

So we can just get the values for  $H_2$ ,  $H_3$ ,  $H_4$  and  $H_5$  directly from the tables for combustion gases. So we will fill out these values. So  $H_2$  cap would be 8.47 kJ/mol and  $H_3$  cap would be 8.12 kJ/mol and  $H_4$  cap would be 32.47 kJ/mol and  $H_5$  cap would be 30.56 kJ/mol. So these

values are the same as what we had obtained for the heat of reaction method. So now the unique thing has to be for H 6 cap and H 7 cap where compounds are involved.

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Example #1

$\hat{H}_6 = (\Delta \hat{H}_f^\circ)_{CO_2} + \hat{H}_a$   
 $= -344.9 \text{ kJ/mol}$

$\hat{H}_6$ : C(s), O<sub>2</sub>(g) at 25°C  
 ↓  
 CO<sub>2</sub>(g) at 1000°C  
 Step 1: C(s) + O<sub>2</sub>(g) → CO<sub>2</sub>(g) at 25°C  
 Step 2: CO<sub>2</sub> at 25°C → CO<sub>2</sub> at 1000°C

So now let us look at H 6 cap. So what is H 6 cap? H 6 cap is for carbon dioxide. So carbon solid which is in the reference state and oxygen gas at 25 degree Celsius which is, this is basically the reference state which we have used, right? So from here it forms carbon dioxide gas at 1000 degree Celsius. So this involves 2 steps. One is the formation of carbon dioxide and the other is the heating of carbon dioxide from 25 degree Celsius to 1000 degree Celsius.

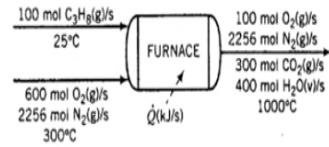
In heat of formation, the standard heat of formation can be obtained for carbon dioxide being produced from carbon solid and oxygen gas at 25 degree Celsius. So this process actually has 2 steps where you have step 1 as carbon solid plus oxygen gas forms carbon dioxide gas where all are at 25 degree Celsius. So this is the first step. Step 2 is where CO<sub>2</sub> at 25 degree Celsius is actually heated to CO<sub>2</sub> at 1000 degree Celsius.

So the first step basically would be the heat of formation obtained for the change in enthalpy. The second step would be integral Cp dT or you can get that value from enthalpy table or the combustion tables. So what you would have here would be H 6 cap would actually be equal to delta H f cap for carbon dioxide plus delta, we will just call it as H a cap where H a cap is

nothing but heating of carbon dioxide from 25 to 1000. So you can get these values from the tables and you would end up with H 6 cap as -344.9 kJ/mol.

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### Example #1



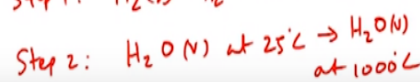
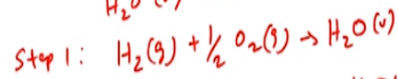
$$\hat{H}_7 = (\Delta \hat{H}_f)_{H_2O(v)} + \hat{H}_b$$

$$\hat{H}_7 = -204.1 \text{ kJ/}$$

$$\hat{H}_7: H_2(g), O_2(g) \text{ at } 25^\circ C$$

$$\downarrow$$

$$H_2O(v) \text{ at } 1000^\circ C$$



Similarly, H 7 cap is basically hydrogen gas and oxygen gas at 25 degree Celsius becoming water vapor at 1000 degree Celsius. So this can be broken down in different ways. So if we have the heat of formation for water vapor itself then it becomes simpler and luckily it is readily available in the tables to get the heat of formation for water vapor and so this standard heat of formation of water vapor at 25 degree Celsius can be obtained from your textbook or other reference books.

So if you were to do this then what you have is step 1 which is nothing but H<sub>2</sub> gas + 1/2 O<sub>2</sub> gas forms H<sub>2</sub>O vapor. So this would be the heat of formation where the change in enthalpy is happening. And the step 2 is where H<sub>2</sub>O vapor at 25 degree Celsius goes to H<sub>2</sub>O vapor at 1000 degree Celsius. So these are 2 different steps which can be accounted for. In case you do not have the heat of formation for water vapor what you would have done is you would have accounted for the heat of formation where water liquid is formed.

So you would have had hydrogen gas + oxygen gas forming water liquid and once you have water liquid at 25 degree Celsius the next step would be from water liquid at 25 degree Celsius to water liquid at 100 degree Celsius. Then the next step would be the heat of vaporization at 100

degree Celsius and then you would have water vapor being heated from 100 to 1000 degree Celsius.

So you would have had a couple of more steps in the hypothetical path which would be built and you would have calculated the values from that, okay? So since we do have the heat of formation for water vapor, we can just use this technique and we will have H 7 cap as heat of formation of water vapor plus I will call this as H b cap which is nothing but integral C p dT of water vapor from 25 to 1000 or you can also get it from the enthalpy table for combustion gases.

So from this you can calculate H 7 cap as -204.1 kJ/mol. So now using these values you can actually fill the enthalpy table.

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Example #1

	$\dot{n}_{in}$	$\hat{H}_{in}$	$\dot{n}_{out}$	$\hat{H}_{out}$
$C_3H_8$	100	-103.8	-	-
$O_2$	600	8.47	100	32.47
$N_2$	2256	8.12	2256	30.56
$CO_2$	-	-	300	-344.9
$H_2O$	-	-	400	-204.1

$\Delta H = -1.26 \times 10^5 \text{ kJ/s}$   
 $\dot{Q} = -126 \times 10^5 \text{ kJ/s}$

So your enthalpy table would now look like this. You would have propane, oxygen, nitrogen, carbon dioxide and water. You have n in dot, H cap in, n out dot and H cap out. So n in is 100, 600 and 2254 and these are 0 and you have n out as zeroes for this and 100, 2256 and 300 and 400. So if you were to plug in the enthalpy values we calculated, we would have H 1 cap as -103.8. The H 2 cap would be 8.47.

This would be 8.12 and you have H 4 cap as 32.47 and this as 30.56 and we also calculated these values as -344.9 and this would be -204.1. So from here we can calculate the total change in



enthalpy like however we have been doing till now. So all you need to do is find the total enthalpy of the outlet streams as the summation of the products of molar flow rates and the specific enthalpy.

And the inlet enthalpy can also be calculated and the difference in these two values would be your total change in enthalpy and if you were to do that you would again get  $\Delta H$  dot as  $-1.26 \times 10^5$  kJ/s which is what your  $Q$  dot would also be. So as you expected, the final values are exactly the same which tells us that both techniques are correct and give us the same values.

But now how did we actually account for heat of reaction here in the heat of formation method? We did not explicitly look at the heat of reaction. We did not account for the reaction. But what we have done is we have implicitly accounted for it by using Hess's law. So as an exercise, please try to solve this and try to see how Hess's law has been applied here to use the reaction while we are performing the energy balances. Try to look at the principles.

Try to see how it has been implemented and do this as an exercise for you to get better understanding of these techniques. I will solve that in the next lecture. But please do try it on your own before you watch the next video. Thank you.