Material and Energy Balances
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Lecture - 57
Fundamentals for Energy Balances on Reactive Processes: Tutorials

Welcome to today's lecture on fundamentals of energy balances on reactive processes. We have already looked at the basic concepts that are required for performing energy balance calculations and today we will be performing tutorial session where we will practice some of the problems which will help us fully understand the concepts which are required for energy balance calculations. Let us start with the tutorial problems. So here is the first problem.

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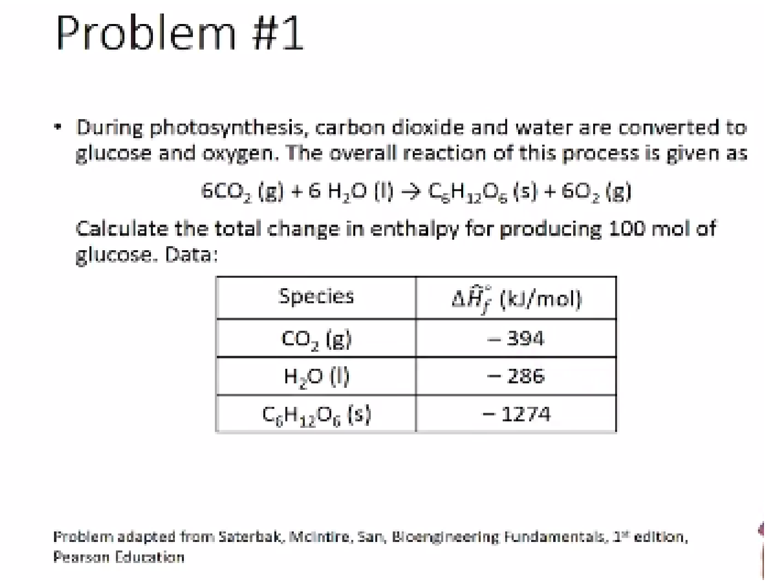

Problem #1

- During photosynthesis, carbon dioxide and water are converted to glucose and oxygen. The overall reaction of this process is given as

$$6CO_2\,(g) + 6\,H_2O\,(l) \rightarrow C_6H_{12}O_6\,(s) + 6O_2\,(g)$$

Calculate the total change in enthalpy for producing 100 mol of glucose. Data:

Species	$\Delta\hat{H}_f^\circ$ (kJ/mol)
CO_2 (g)	− 394
H_2O (l)	− 286
$C_6H_{12}O_6$ (s)	− 1274

Problem adapted from Saterbak, McIntire, San, Bioengineering Fundamentals, 1st edition, Pearson Education

During photosynthesis, carbon dioxide and water are converted to glucose and oxygen. The overall reaction of this process is given as 6 moles of carbon dioxide reacts with 6 moles of water to form 1 mole of glucose and 6 moles of oxygen. You are asked to calculate the total change in enthalpy for producing 100 moles of glucose. The data given to you is the heat of formation for carbon dioxide, water and glucose.

So you have not been given a heat of formation for oxygen because that would be 0. Oxygen gas is the elemental component present in its native state which would mean the heat of formation for this particular component would be 0. So we have these heats of formations and we have to calculate the total change in enthalpy for producing 100 moles of glucose. This information can be obtained once we know the heat of reaction.

The heat of reaction can be calculated using the heats of formations that have been provided to us. Let us look at the heat of formation component and let us try to apply the equation which is built on Hess's law.

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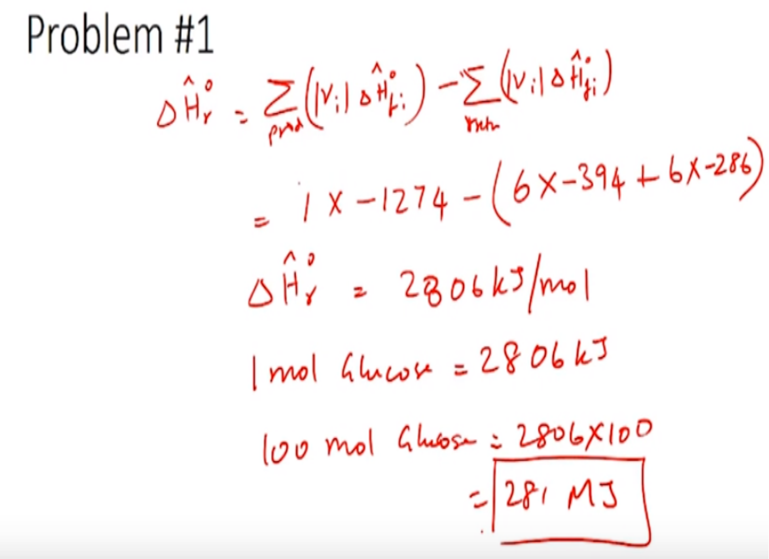

Problem #1

$$\Delta \hat{H}_r^o = \sum_{prod}\left(|\nu_i| \Delta \hat{H}_{f_i}^o\right) - \sum_{rxn}\left(|\nu_i| \Delta \hat{H}_{f_i}^o\right)$$

$$= 1 \times -1274 - (6 \times -394 + 6 \times -286)$$

$$\Delta \hat{H}_r^o = 2806 \, kJ/mol$$

1 mol Glucose = 2806 kJ

100 mol Glucose = 2806×100

$$= \boxed{281 \, MJ}$$

So the equation for heat of reaction would be sigma of products (nu i delta H f i) where H f is the heat of formation and nu i is the stoichiometric coefficient minus sigma of reactants (nu i delta H f i cap). So this is the equation which you have derived using Hess's law and we have already checked if this equation is valid. So we can test it one more time while we are doing the calculations.

Heat of reaction can be calculate using this equation as the stoichiometric coefficient of the product which is glucose 1 times the heat of formation for glucose which is given as -1274 minus stoichiometric coefficient of carbon dioxide which is one of the reactants 6 times the heat of formation of carbon dioxide which is -394 + 6 times -286 which is the stoichiometric coefficient and heat of formation for water.

So using this we can calculate the heat of reaction as 2806 kJ/mol. While 1 mole of glucose is produced, the total change in enthalpy for this process would be 2806 kJ. So we have been asked to calculate this for 100 moles of glucose. This would be 2806 times 100 which = 281 MJ. So this would be roughly the total amount of change in enthalpy for the process where we produce 100 moles of glucose.

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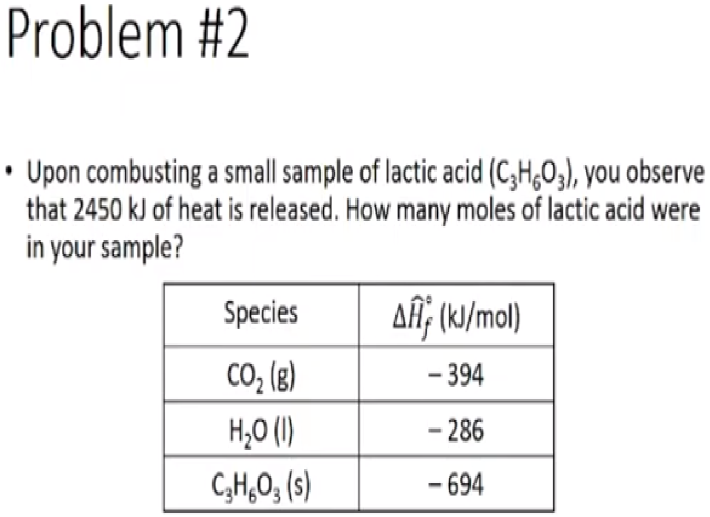

Problem #2

- Upon combusting a small sample of lactic acid ($C_3H_6O_3$), you observe that 2450 kJ of heat is released. How many moles of lactic acid were in your sample?

Species	$\Delta \hat{H}_f^\circ$ (kJ/mol)
CO_2 (g)	– 394
H_2O (l)	– 286
$C_3H_6O_3$ (s)	– 694

Let us now look at a different problem. So here instead of asking us to calculate change in enthalpy we have been asked to calculate amount and let us see what exactly the problem is. Upon combusting a small sample of lactic acid you observe that 2450 kJ of heat is released. How many moles of lactic acid were there in your sample? So you have been given the heat of formations again.

Heat of formation for carbon dioxide and water has been given and the heat of formation for lactic acid has also been provided to you. Now, we need to identify what would be the number of moles of lactic acid combusted so that there is a heat of 2450 kJ being released. For this we need to know the heat of combustion for lactic acid. How would we calculate the heat of combustion. For this we first need to write down the combustion reaction and identify what are the components which are present in the combustion reaction. So let us look at this process.

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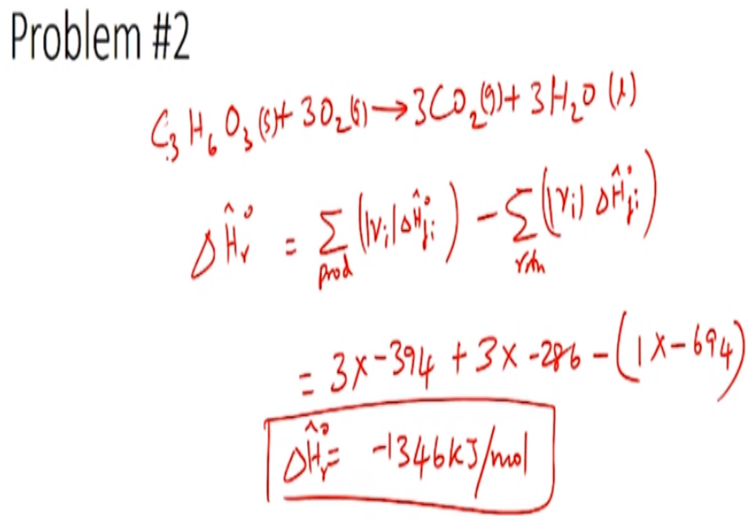

Problem #2

$$C_3H_6O_3(s) + 3O_2(g) \rightarrow 3CO_2(g) + 3H_2O(l)$$

$$\Delta\hat{H}_r^\circ = \sum_{prod}\left(|\nu_i|\Delta\hat{H}_{fi}^\circ\right) - \sum_{rxn}\left(|\nu_i|\Delta\hat{H}_{fi}^\circ\right)$$

$$= 3\times-394 + 3\times-286 - \left(1\times-694\right)$$

$$\boxed{\Delta\hat{H}_r^\circ = -1346\,kJ/mol}$$

The combustion reaction for lactic acid would be C3H6O3 + oxygen gives CO2 + H2O. So because we have the heat of formation for water, let us assume the product of this combustion is also water liquid. So making that assumption let us now balance this equation. We have 3 atoms of carbon coming in. So we will have to have 3 atoms of carbon leaving. So it will be 3 moles of carbon dioxide produced. We have 6 atoms of hydrogen entering.

So 6 atoms of hydrogen has to leave the reaction thereby having 3 moles of water being produced and finally we now have to balance the oxygen. So now that we have balanced both these components in the product side let us see how many moles of oxygen is present. We have 3 times 2, 6 + 3 times 1, 9. 9 atoms of oxygen is present in the product side. So we have 3 of that in the lactic acid. So the other 6 has to come from the oxygen.

So 3 moles of oxygen molecule reacts with 1 mole of lactic acid to produce 3 moles of carbon dioxide and 3 moles of water. So we are assuming water liquid, carbon dioxide gas, oxygen gas and lactic acid solid because we have the information for these phases directly. If you were to assume the water which is being produced as water vapor then we would have to use the heat of vaporization and include that as part of the heat of formation calculations.

So we will try to do that as well but right now we will first use this assumption and perform the calculations. So because this equation is there we have the heat of formation for lactic acid, carbon dioxide and water we can calculate the heat of this reaction which is the combustion reaction again using Hess's law, the equation would be sigma of products nu i delta H f cap – sigma of reactants nu i delta H f i and this would be given to us.

These values for the heat of formations have been given. So the products are carbon dioxide and water. So this would be 3 times the heat of formation of carbon dioxide which is -394 + 3 times the heat of formation of water liquid which is -286 – 1 times which is the stoichiometric coefficient of lactic acid times the heat of formation of lactic acid which is -694 and this would give us the heat of reaction as -1346 kJ/mol.

So this would be the heat of combustion for lactic acid if it were producing water liquid. In case we have water vapor as the product component then what would be the heat of combustion? Let us try to calculate that as well.

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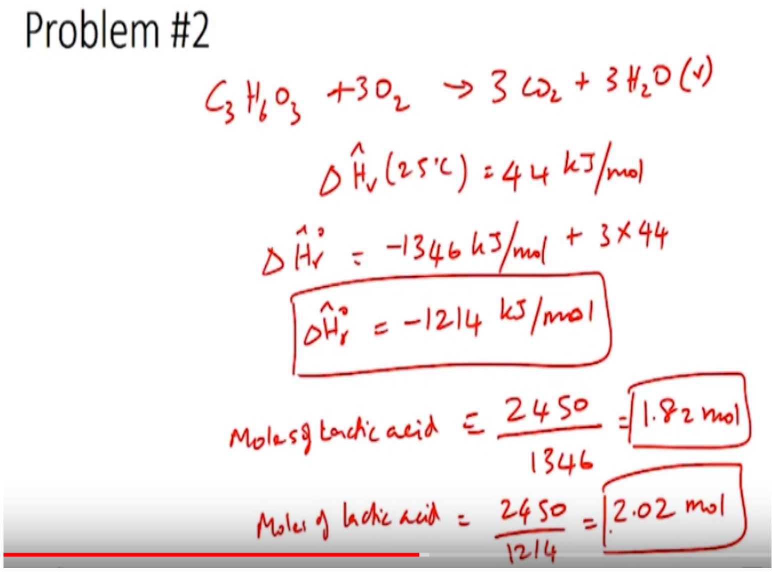

Problem #2

$$C_3H_6O_3 + 3O_2 \rightarrow 3CO_2 + 3H_2O(v)$$

$$\Delta \hat{H}_v(25^\circ C) = 44 \text{ kJ/mol}$$

$$\Delta \hat{H}_r^\circ = -1346 \text{ kJ/mol} + 3 \times 44$$

$$\boxed{\Delta \hat{H}_r^\circ = -1214 \text{ kJ/mol}}$$

$$\text{Moles of lactic acid} = \frac{2450}{1346} = \boxed{1.82 \text{ mol}}$$

$$\text{Moles of lactic acid} = \frac{2450}{1214} = \boxed{2.02 \text{ mol}}$$

Now, if we were to consider a reaction where water vapor is the product. So you would have C3H6O3 + 3O2 forming 3CO2 + 3 H2O. Here it would be a vapor. So what happens is the heat of reaction will have to change to account for this heat of vaporization. The heat of vaporization for water at 25 degree Celsius is 44 kJ/mol. So since we have 3 moles of water being evaporated in the product side, we have to account for that appropriately.

Heat of reaction has to be calculated by including the heat of vaporization. As the heat of reaction is defined as the enthalpy of products minus the enthalpy of reactants here the enthalpy of products has actually increased because of the heat of vaporization. So we will be adding this heat of vaporization times the number of moles of water which is being vaporized to the heat of reaction to get the actual heat of reaction for this process.

So that would be -1346 kJ/mol + 3 times 44 giving you a value of -1214 kJ/mol. So this would be the heat of reaction if water vapor is being formed. To identify the total number of moles of lactic acid which has actually been combusted in the system we have, we have to use either the heat of combustion based on water liquid being formed or water vapor being formed and let us assume one of them as the situation.

We will assume, in this case I have assumed that water liquid is being formed to calculate the total number of moles of lactic acid which is burnt in this process. So that would mean moles of lactic acid combusted would be equal to 2450/1346 which is the 1346 kJ is the amount of heat which would be released when 1 mole of lactic acid is burnt. This would give us a value of 1.82 moles.

So if we have water liquid as the final combustion product then we would have 1.82 moles of lactic acid burnt. If it were water vapor which is in the final product, then the equation would be 2450/1214 which would be roughly 2.02 moles. So we approximately have about 1.82 moles of lactic acid which is being burnt to produce carbon dioxide and water and this is calculated based on the heat of reaction which we obtained using the heats of formations.

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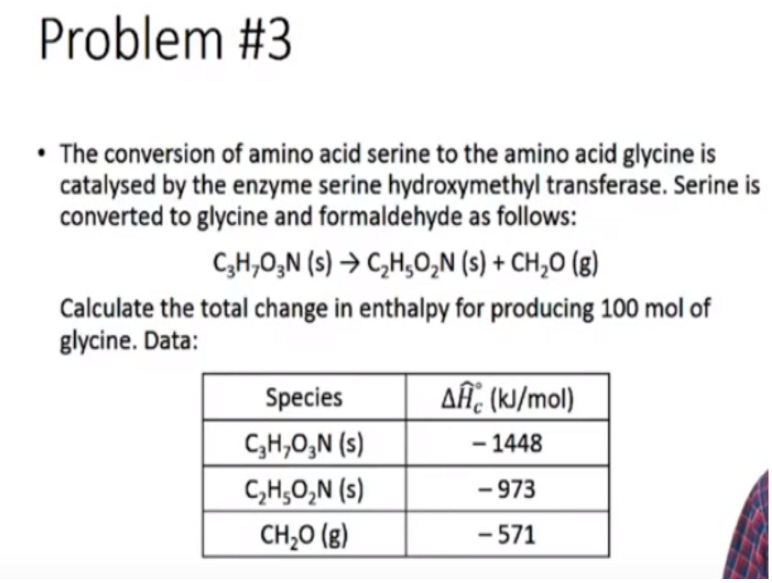

Problem #3

- The conversion of amino acid serine to the amino acid glycine is catalysed by the enzyme serine hydroxymethyl transferase. Serine is converted to glycine and formaldehyde as follows:

$$C_3H_7O_3N\ (s) \rightarrow C_2H_5O_2N\ (s) + CH_2O\ (g)$$

Calculate the total change in enthalpy for producing 100 mol of glycine. Data:

Species	$\Delta \hat{H}_c^\circ$ (kJ/mol)
$C_3H_7O_3N$ (s)	− 1448
$C_2H_5O_2N$ (s)	− 973
CH_2O (g)	− 571

Now let us look at the third example problem. So here we have conversion of an amino acid serine to another amino acid which is glycine catalyzed by an enzyme called serine hydroxymethyl transferase. Serine is converted to glycine and formaldehyde as shown in the reaction. So you have to calculate the total change in enthalpy for producing 100 moles of glycine. So here you have been given the heat of combustion. So how do we use heat of combustion to calculate the heat of reaction?

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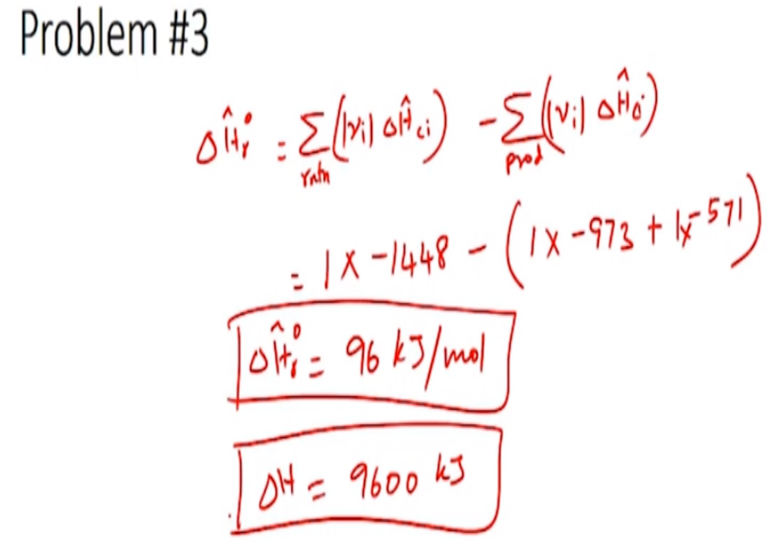

Problem #3

$$\Delta \hat{H}_r^\circ = \sum_{rxn} \left(|\nu_i|\, \Delta \hat{H}_{ci}\right) - \sum_{prod} \left(|\nu_i|\, \Delta \hat{H}_{c}^{\circ}\right)$$

$$= 1 \times -1448 - \left(1 \times -973 + 1 \times -571\right)$$

$$\boxed{\Delta \hat{H}_r^\circ = 96\ \text{kJ/mol}}$$

$$\boxed{\Delta H = 9600\ \text{kJ}}$$

We have already looked at this in the earlier lecture. So we can use Hess's law and the equation for heat of reaction using combustion enthalpy. Heat of combustion would be sigma of reactants (nu i delta H cap c i) – sigma of products (nu i delta of H cap c i). So this would be the total change in enthalpy of the heat of reaction for the process. For the equation that has been given, the reactant is serine and the products are glycine and formaldehyde.

So the reactant serine would have heat of combustion that has been given. So the stoichiometric coefficient is 1 times the heat of combustion which is -1448 minus the products which are glycine and formaldehyde. So both are 1 moles only. So 1 times -973 - sorry + 1 times -571. So this would be equal to 96 kJ/mol. So the heat of reaction for this process, for this particular process where serine is converted to glycine is 96 kJ/mol.

We have been asked to calculate the change in enthalpy for 100 moles of glycine being produced. So that would mean delta H would be equal to 9600 kJ. So this is the final answer we are looking for.

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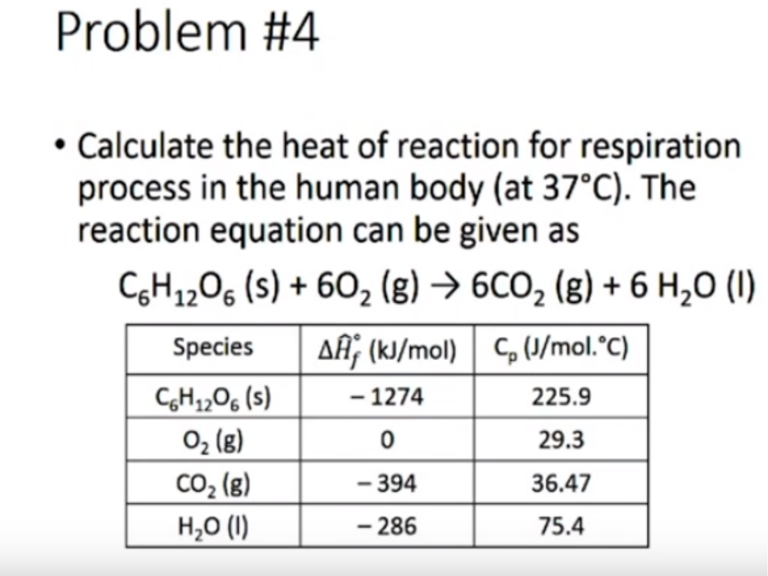

Problem #4

- Calculate the heat of reaction for respiration process in the human body (at 37°C). The reaction equation can be given as

$$C_6H_{12}O_6\,(s) + 6O_2\,(g) \rightarrow 6CO_2\,(g) + 6\,H_2O\,(l)$$

Species	$\Delta\hat{H}_f^\circ$ (kJ/mol)	C_p (J/mol.°C)
$C_6H_{12}O_6$ (s)	– 1274	225.9
O_2 (g)	0	29.3
CO_2 (g)	– 394	36.47
H_2O (l)	– 286	75.4

Here is the fourth problem for this tutorial session. You are asked to calculate the heat of reaction for respiration process in the human body which happens at 37 degree Celsius. The reaction equation can be given as glucose + oxygen gives carbon dioxide and water. So this reaction is happening at 37 degree Celsius. Until now we have been calculating the standard heat of reaction which is at 25 degree Celsius.

So the information given to us here is also standard heat of formation which is what is readily available in tables and textbooks. So using this we can actually calculate only the heat of reaction for 25 degree Celsius which would be the standard heat of reaction. How do we calculate the heat of reaction at 37 degree Celsius? So this is a simple problem which we can solve if we were to apply principles which we have learnt earlier. You will have to build a hypothetical path.

The hypothetical path which you would build will be the reactants which are at 37 degree Celsius in your body would have to be cooled to 25 degree Celsius and the reaction itself will happen at 25 degree Celsius so that you can use the heat of reaction that you calculate and the products which are formed at 25 degree Celsius would then have to be heated to 37 degree Celsius. So now instead of having a single step, you actually have 3 steps.

So you would have to build this hypothetical path and calculate the change in enthalpy for individual steps and thereby calculate the total change in enthalpy for the process which would be the heat of reaction for the given reaction at 37 degree Celsius. Let us go ahead and solve this problem.

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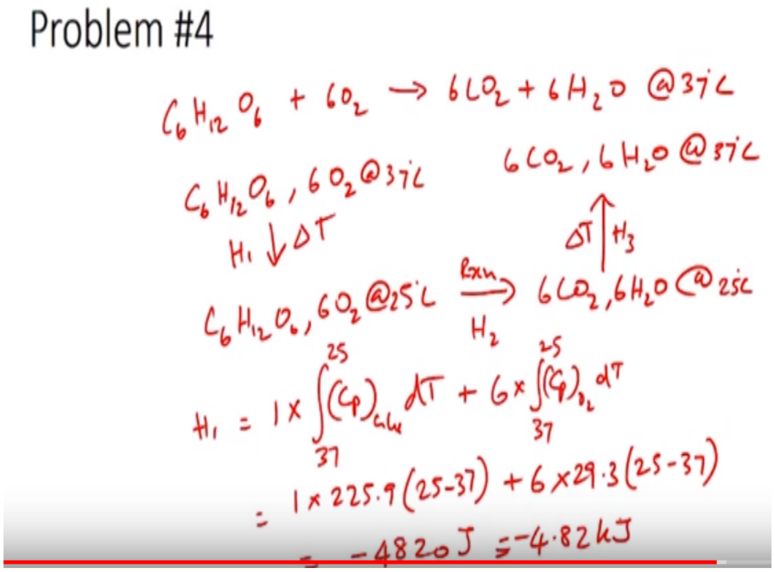

Problem #4

$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$ @37°C

$$\begin{tikzcd} C_6H_{12}O_6, 6O_2 \text{@}37^\circ C \arrow[d, "H_1"', "\Delta T"] & 6CO_2, 6H_2O \text{@}37^\circ C \\ C_6H_{12}O_6, 6O_2 \text{@}25^\circ C \arrow[r, "Rxn", "H_2"'] & 6CO_2, 6H_2O \text{@}25^\circ C \arrow[u, "\Delta T", "H_3"'] \end{tikzcd}$$

$$H_1 = 1 \times \int_{37}^{25} (C_p)_{Glu}\, dT + 6 \times \int_{37}^{25} (C_p)_{O_2}\, dT$$

$$= 1 \times 225.9(25-37) + 6 \times 29.3(25-37)$$

$$= -4820\ J = -4.82\ kJ$$

As I said, we have to look at a hypothetical path. So the actual process which we are looking at is C6 H12 O6 + 6O2 gives 6 CO2 + 6H2O. This is happening at 37 degree Celsius. So this is the real reaction which is happening. So this means reactants at 37 degree Celsius are reacting to form products at 37 degree Celsius. So instead we are going to change this into a hypothetical path where you have reactants glucose and 6 moles of oxygen being cooled, which are at 37 degree Celsius are being cooled to reactants at 25 degree Celsius.

So here it is forming products which would be 6CO2 and 6H2O all at 25 degree Celsius. And from here it is being heated to form the products at 37 degree Celsius. So now, the first step is only temperature changing. The second step is the reaction. The third step is again only temperature changing. So we can calculate the change in enthalpy for the first step. Let us call that H 1 cap and this would be H 2 cap and this would be H 3 cap.

H 1 cap can be calculated as integral C p dT and we will basically be able to calculate the total change in enthalpy for this process for 1 mole of glucose and 6 moles of oxygen which would be H 1 and this would be H 2 which would be the heat of reaction for this process and you will have H 3 which is for heating of carbon dioxide and water, 6 moles of each to reach 37 degree Celsius. Let us see how we go about solving this problem. H 1 would be equal to two things.

One is glucose being cooled from 37 to 25 and the other is 6 moles of oxygen being cooled from 37 to 25. So for calculating the enthalpy change associated with cooling 1 mole of glucose, we would have to find, calculate 1 times integral C p of glucose dT where temperature changes from 37 to 25 plus the enthalpy change associated with cooling 6 moles of oxygen would be 6 times integral C p of oxygen dT and this is again cooling from 37 to 25.

So this would be 1 times 225.9 times 25 – 37 + 6 times 29.3 times 25 -37 and this value is -4820 J or equivalent to -4.82 kJ. So this is the first step. Now, for calculating the heat of reaction for this process, the second step, the standard heat of reaction can be calculated using the heats of formation that have been given. However, I am not going to go through the calculations here. This is just the reverse of the reaction which we have looked at.

So we can easily do this calculation. So I will just give a one line explanation for what we are doing.

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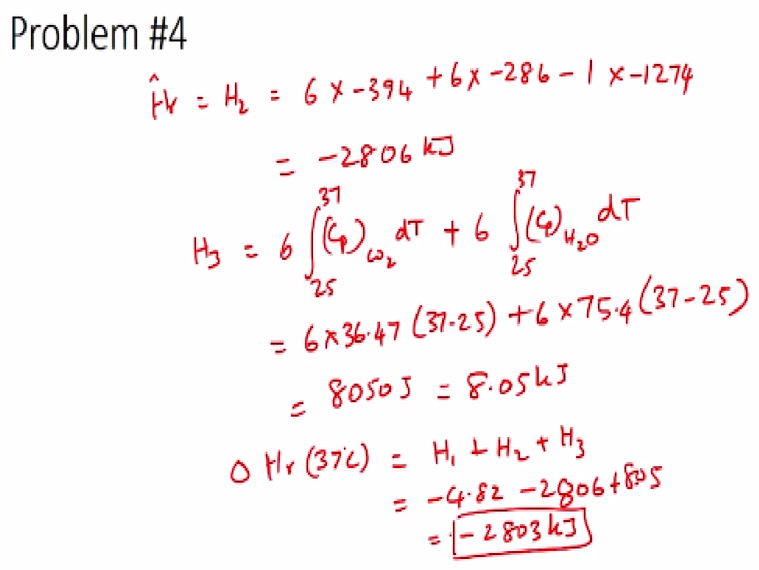

Problem #4

$$\hat{H}_r = H_2 = 6 \times -394 + 6 \times -286 - 1 \times -1274$$

$$= -2806 \text{ kJ}$$

$$H_3 = 6\int_{25}^{37} (C_p)_{CO_2}\, dT + 6\int_{25}^{37} (C_p)_{H_2O}\, dT$$

$$= 6 \times 36.47\,(37-25) + 6 \times 75.4\,(37-25)$$

$$= 8050\text{ J} = 8.05\text{ kJ}$$

$$O H_r(37°C) = H_1 + H_2 + H_3$$

$$= -4.82 - 2806 + 8.05$$

$$= \boxed{-2803\text{ kJ}}$$

So the heat of reaction which is equal to the H2 = 6 times -394 + 6 times -286 – 1 times -1274 giving us a value of -2806 kJ. And the next step we have, H3 would be equal to, again we are now heating 6 moles of carbon dioxide and 6 moles of water from 25 degree Celsius to 37 degree Celsius. So for carbon dioxide it will be 6 times integral C p of carbon dioxide dT from 25 to 37 + 6 times so this second term would be for water.

So from 25 to 37 C p of water dT. And this would be 6 times 36.47 times 37 – 25 + 6 times 75.4 times 37 – 25 giving you a value of 8050 J or = 8.05 kJ. So now the total change in enthalpy for the reaction, the total heat of reaction at 37 degree Celsius would be H 1 + H 2 + H 3 which would be equal to -4.82 – 2806 – 8.05 sorry + 8.05 giving you a value of -2803 kJ. So this would be heat of reaction for the given reaction which happens as respiration process in your body at 37 degree Celsius.

So with this we have come to the end of the tutorial session for covering the fundamentals associated with energy balances involving reactions. In the next lecture, we will look at solving energy balance problems that have reactions in them. We will look at what techniques can be used and we will solve more example problems which will help us familiarize with these concepts. Until then thank you and good bye.