Basic Principles and Calculations in Chemical Engineering
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Lecture - 25
Energy Balance With Heat of Reaction (Contd..)

Welcome to massive open online course on basic principles and calculations in chemical engineering. We are discussing about energy balances on reactive system under module eight. Now in this module, the lecture 8.2 we will discuss about energy balance with heat of reaction, which is continuation of the previous lecture.

There we have described about different you know aspect of energy balances on heat of reaction based on heat of formation and also we have described those heat of reaction based on heat of formation with different examples.

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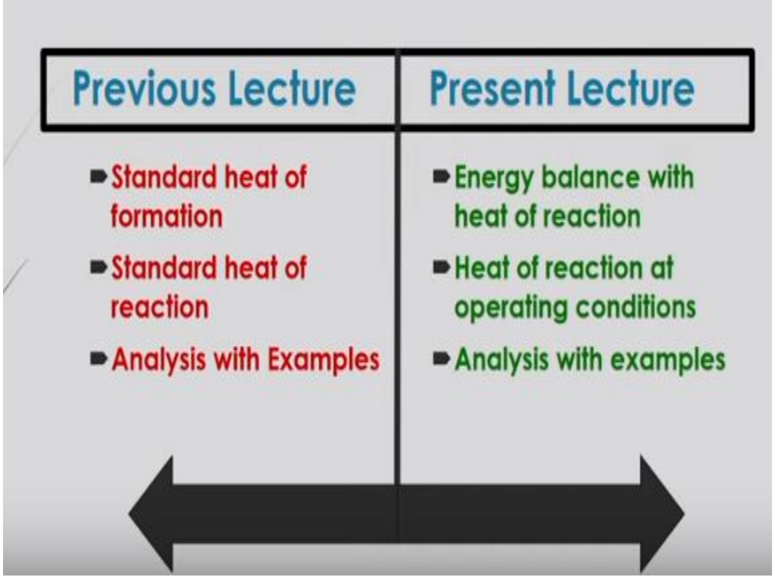

Previous Lecture	Present Lecture
Standard heat of formation	Energy balance with heat of reaction
Standard heat of reaction	Heat of reaction at operating conditions
Analysis with Examples	Analysis with examples

Now in this lecture we will describe more about that energy balances with heat of reaction and this heat of reaction will be based on that at operating conditions with some examples there.

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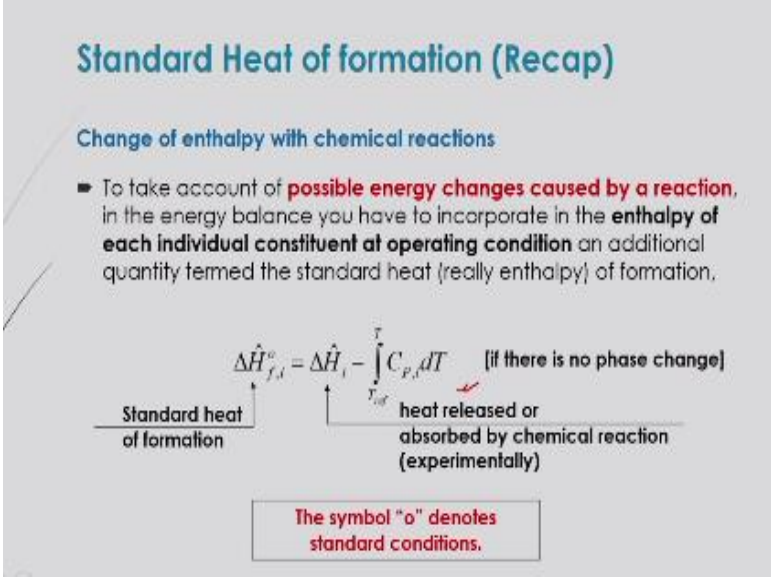

Standard Heat of formation (Recap)

Change of enthalpy with chemical reactions

- To take account of **possible energy changes caused by a reaction**, in the energy balance you have to incorporate in the **enthalpy of each individual constituent at operating condition** an additional quantity termed the standard heat (really enthalpy) of formation.

$$\Delta \hat{H}^o_{f,i} = \Delta \hat{H}_i - \int_{T_{ref}}^{T} C_{p,i}\, dT$$

[if there is no phase change]

Standard heat of formation

heat released or absorbed by chemical reaction (experimentally)

The symbol "o" denotes standard conditions.

Now let us look back of that you know standard heat of formation based on which you can calculate the standard heat of reaction, which is very important for calculation of heat of reaction at any operating condition. Now what is that standard heat of formation?

This is basically the formation of that constituents which are taking part in a particular reaction and at the standard condition how these constituents are formed by you know absorbing energy or releasing energy. So those amount of energy which is released or adsorbed by formation of that constituent is called heat of formation at the standard condition.

Now that heat of formation can be calculated based on that reaction, you know enthalpy change or energy changed due to that reaction and which can be obtained experimentally and based on that experimental data this heat of formation can be calculated for that individual components which are actually taking part in that particular reaction.

So we have described already this you know equation to calculate that heat of formation for particular constituents.

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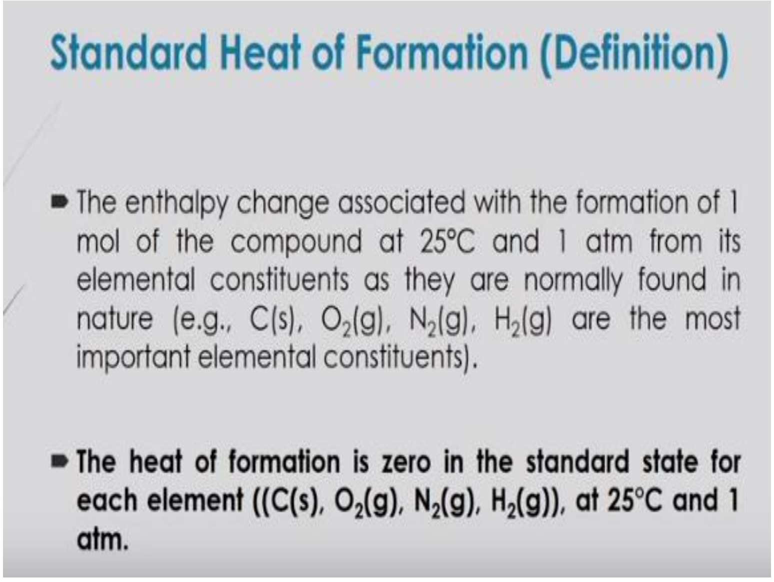

Standard Heat of Formation (Definition)

- The enthalpy change associated with the formation of 1 mol of the compound at 25°C and 1 atm from its elemental constituents as they are normally found in nature (e.g., $C(s)$, $O_2(g)$, $N_2(g)$, $H_2(g)$ are the most important elemental constituents).
- **The heat of formation is zero in the standard state for each element (($C(s)$, $O_2(g)$, $N_2(g)$, $H_2(g)$), at 25°C and 1 atm.**

Now since this is the enthalpy change which is associated with the formation of one mole of the compound at 25 degrees Celsius and one atmosphere from its elemental constituents. Now in the nature you will see that some components will be you know occurring automatically or you can say that just in nature in an you know elemental forms or some molecular forms like that oxygen, nitrogen, hydrogen etc.

Even some elemental forms like carbon there. So for those cases that standard heat of formation will be considered as a zero there. So you have to you know, consider that enthalpy change because of this, you know elemental constituents or this you know molecular you know form in the nature that will be you know considered as a heat of formation of zero.

But other compound which are formed during the reaction based on these elements and also other you know naturally occurring compounds. For that, you have to you know find out what should be the heat of formation at that particular operating condition as well as what will be the you know heat of formation at standard condition that you have to consider.

And based on that heat of formation, that heat of reaction to be calculated and also this standard heat of reaction to be added whenever there will be a certain process and if you have the change of enthalpy or energy change because of that you know production of that some substances by the reaction.

And considering that reactants there and based on that enthalpy change of that reactants and products, what should be the you know energy change along with that, you know a standard heat of reaction that you have to consider for that standard heat of reaction at a particular operating condition.

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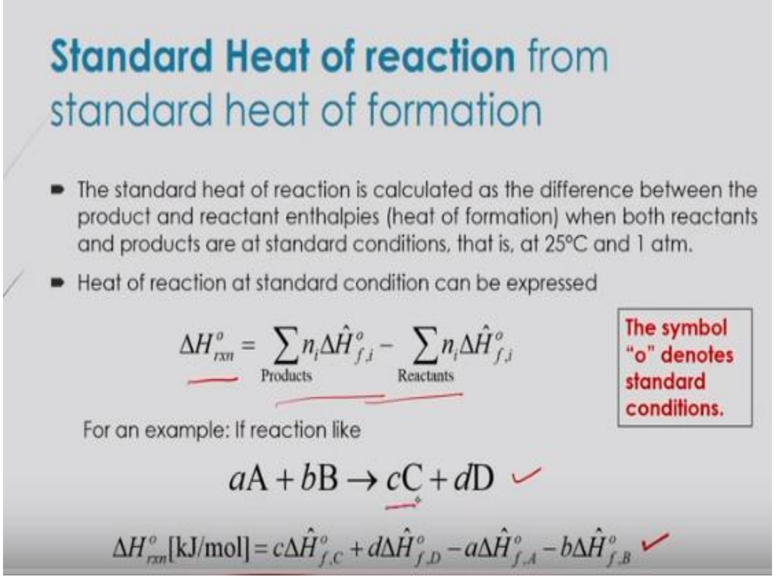

Standard Heat of reaction from standard heat of formation

- The standard heat of reaction is calculated as the difference between the product and reactant enthalpies (heat of formation) when both reactants and products are at standard conditions, that is, at 25°C and 1 atm.
- Heat of reaction at standard condition can be expressed

$$\Delta H^o_{rxn} = \sum_{\text{Products}} n_i \Delta\hat{H}^o_{f,i} - \sum_{\text{Reactants}} n_i \Delta\hat{H}^o_{f,i}$$

The symbol "o" denotes standard conditions.

For an example: If reaction like

$$aA + bB \rightarrow cC + dD$$

$$\Delta H^o_{rxn}[\text{kJ/mol}] = c\Delta\hat{H}^o_{f,C} + d\Delta\hat{H}^o_{f,D} - a\Delta\hat{H}^o_{f,A} - b\Delta\hat{H}^o_{f,B}$$

Now since we have described that to how to you know calculate the standard heat of reaction at that 25 degree Celsius and one atmospheric condition, we have you know given this equation here like you know delta H you know rxn 0 this zero means here that denotes standard conditions and rxn means reaction.

So this standard heat of reaction is basically what will be the change of you know enthalpy of formation of each constituents in the products and reactants. And this already described in the previous you know lecture that this heat of reaction can be calculated based on this equation when there is a reaction is aA + bB that will give you that products of you know C and D with that stoichiometric coefficient of you know C and D.

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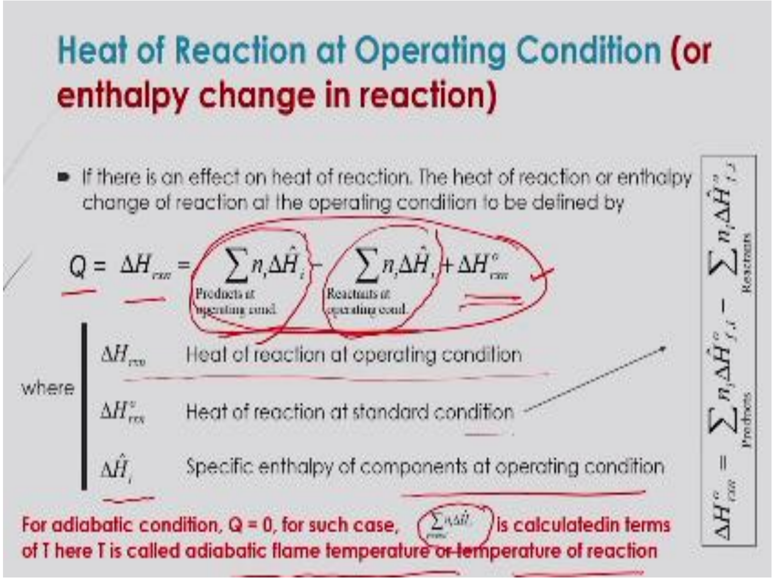

Heat of Reaction at Operating Condition (or enthalpy change in reaction)

- If there is an effect on heat of reaction. The heat of reaction or enthalpy change of reaction at the operating condition to be defined by

$$Q = \Delta H_{rxn} = \sum_{\substack{\text{Products at}\\\text{operating cond.}}} n_i \Delta \hat{H}_i - \sum_{\substack{\text{Reactants at}\\\text{operating cond.}}} n_i \Delta \hat{H}_i + \Delta H^{\circ}_{rxn}$$

where

ΔH_{rxn} Heat of reaction at operating condition

ΔH°_{rxn} Heat of reaction at standard condition

$\Delta \hat{H}_i$ Specific enthalpy of components at operating condition

$$\boxed{\Delta H^{\circ}_{rxn} = \sum_{\text{Products}} n_i \Delta \hat{H}^{\circ}_{f,i} - \sum_{\text{Reactants}} n_i \Delta \hat{H}^{\circ}_{f,i}}$$

For adiabatic condition, Q = 0, for such case, $\sum n_i \Delta \hat{H}$ is calculatedin terms of T here T is called adiabatic flame temperature ~~or~~ temperature of reaction

Now in this case, what should be the heat of reaction other than that standard heat of standard heat sorry standard you know condition like at operating condition other than standard you know temperature and pressure. So in that case, if there is an effect on heat of reaction, the heat of reaction or enthalpy change of reaction at that operated condition to be defined by this equation as given in the slides here.

So that heat of reaction will be released as Q and that is basically the change of you know enthalpy during that reaction. And that is actually calculated based on this you know enthalpy change in the you know product as well as you know reactants at that operating conditions along with that you know standard he talked reaction.

So this component here in this reaction, you will be able to you know calculate that summation of you know all enthalpy change at that operating condition for that you know product components and this will be that you know enthalpy change for all components in the reactants. And the subtraction will give you that enthalpy change because of that reaction at that operating condition.

But you have to add what will be the standard heat of formation that with this change of this enthalpy. So if you add this standard heat of reaction finally you know you will get that net you know enthalpy change due to this you know heat of due to this you know operating condition for this reaction.

Now here data H rxn this is basically heat of reaction at operating condition. Delta H rxn is basically heat of reaction at standard condition and also delta H hat i, this is basically specific enthalpy of components at operating condition. Now for adiabatic condition, this Q should be equals to zero.

For such cases this summation of n i delta H hat i is calculated in terms of temperature here. Here T is called that adiabatic flame temperature or temperature of reaction. So at a certain temperature you will see that the change of this you know enthalpy for this you know component i then you have to find out at which temperature this will happen then that temperature to be found out and it is to be actually considered as a flame temperature.

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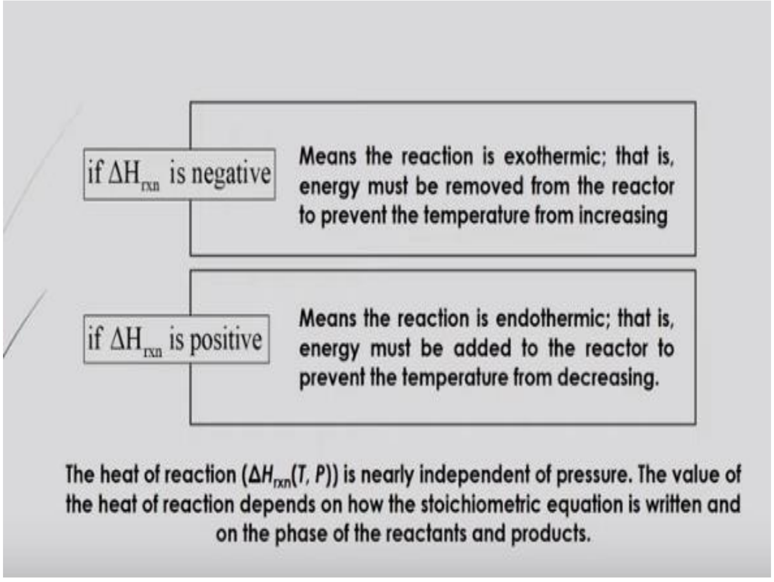

if ΔH_{rxn} is negative — Means the reaction is exothermic; that is, energy must be removed from the reactor to prevent the temperature from increasing

if ΔH_{rxn} is positive — Means the reaction is endothermic; that is, energy must be added to the reactor to prevent the temperature from decreasing.

The heat of reaction ($\Delta H_{rxn}(T, P)$) is nearly independent of pressure. The value of the heat of reaction depends on how the stoichiometric equation is written and on the phase of the reactants and products.

And overall if you have that heat of reaction at that particular operating condition as negative, it will actually reflect that reaction will be as exothermic and in that case energy must be removed from the reactor to prevent that temperature from the increasing based on this reaction.

And if this enthalpy change is positive, that will you know refer to that reaction will be endothermic. In that case, energy must be added to the reactor to prevent the temperature from decreasing. Now the heat of reaction is nearly independent of pressure at that particular you know temperature and pressure you will say.

The value of the heat of reaction depends on how the stoichiometric equation is written and on the phase of the reactants and products are there. So based on this you can calculate what should be the heat of reaction.

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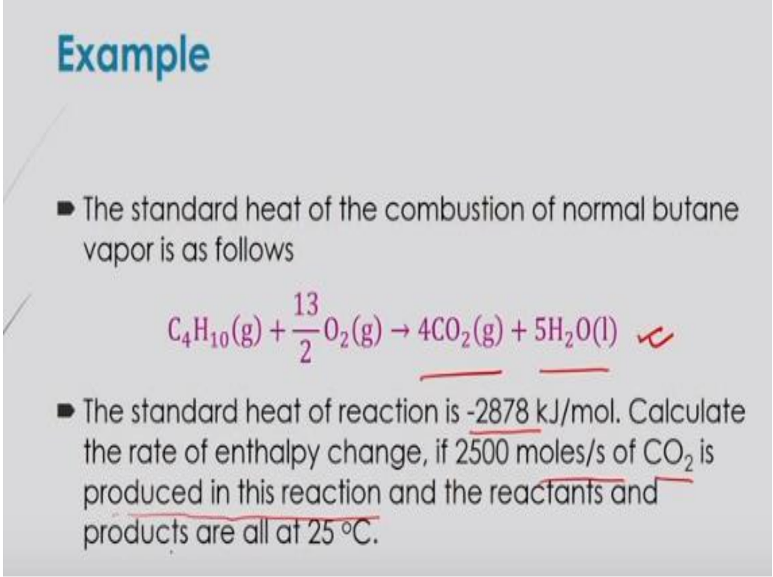

Example

- The standard heat of the combustion of normal butane vapor is as follows

$$C_4H_{10}(g) + \frac{13}{2}O_2(g) \rightarrow 4CO_2(g) + 5H_2O(l)$$

- The standard heat of reaction is -2878 kJ/mol. Calculate the rate of enthalpy change, if 2500 moles/s of CO_2 is produced in this reaction and the reactants and products are all at 25 °C.

Now let us do an example for this theory. In this case we have given that a standard heat of combustion of normal butane vapor as per this you know reaction equation here C 4 H 10 that is in gaseous form. That will you know be burned with that oxygen here and after burning you will see that the carbon dioxide and moisture will be you know coming out.

So in that case, the standard heat of reaction is found that -2878 kilojoule per mole. Now you have to calculate the rate of enthalpy change if 2500 moles per second of carbon dioxide is produced in this reaction and the reactants and products are all at 25 degree Celsius. So how to solve this equation here? Let us solve this equation.

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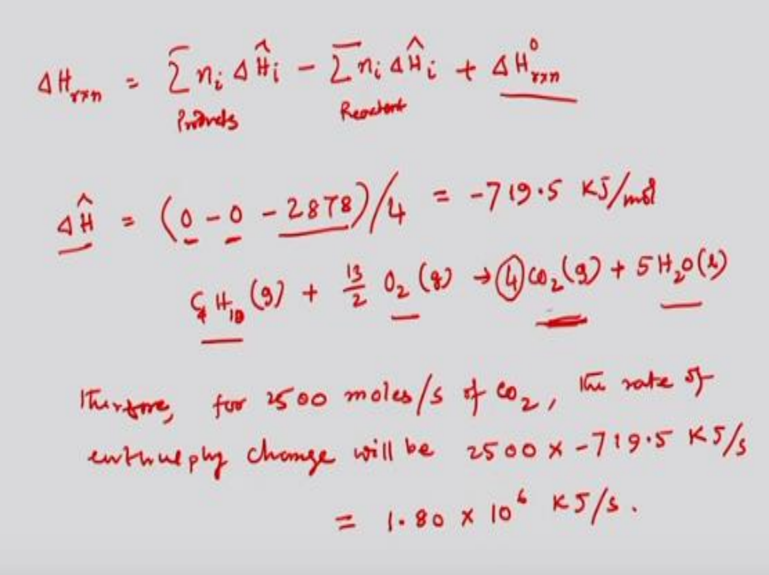

$$\Delta H_{rxn} = \sum_{\text{Products}} n_i \Delta \hat{H}_i - \sum_{\text{Reactant}} n_i \Delta \hat{H}_i + \underline{\Delta H^{0}_{rxn}}$$

$$\underline{\Delta \hat{H}} = (\underline{0} - \underline{0} - \underline{2878})/4 = -719.5 \text{ KJ/mol}$$

$$\underline{C_4H_{10}}(g) + \frac{13}{2}\underline{O_2}(g) \rightarrow \textcircled{4}\underline{CO_2}(g) + 5\underline{H_2O}(l)$$

Therefore, for 2500 moles/s of CO_2, the rate of enthalpy change will be 2500×-719.5 KJ/s

$= 1.80 \times 10^{6}$ KJ/s.

In this case, we know that here the delta H you know rxn that is heat of reaction, that is summation of n i, this is number of ith components into delta H i hat minus summation of here n i delta H hat i. This is in you know that reactant side reactants and these are all products and then you have to add the standard heat of reaction that is delta H rxn at standard condition.

For standard condition it is zero. So enthalpy change at the standard condition for products and reactants are zero. We always you know consider these things that therefore, per mole of carbon dioxide production, the rate of you know change of enthalpy will be delta H hat.

This is specific terms, that will be equal to you know that this is zero, then minus zero minus here 2878 divided by 4. Why it is coming because we know that reaction is what? In this case C 4 H 10 that is in you know gaseous form and plus 13 by 2 O 2 here in gas. That will give you 4 moles of carbon dioxide in gaseous forms plus you know 5 moles of water in liquid form.

So based on this reactions we are getting that since here product side is carbon dioxide and water. So in this case, you will see that this product side here all are you know naturally occurring substance. So here this enthalpy change will be equals to zero for these components and for these components it will be zero.

So finally, what is that you will see that summation of all these you know product components enthalpy at that condition will be equals to zero. That is why here this zero is coming. Similarly for you know that this reactants, similar for reactants you will see that here it is coming that this oxygen is naturally occurring.

And this is also butane, naturally occurring that is in gaseous substance that then enthalpy change will be equals to zero. That is why it is coming as zero. Now another terms is here heat of reaction is given that is -2878. So if you add it then it will be coming this.

Now this is basically based on that one mole you know per mole if you are considering that specific enthalpy change then you have to divide it by the stoichiometric coefficient of carbon dioxide. So it is that is why here 4 there. So based on this you can say that here it is coming after calculation -719.5 kilojoule per mole.

Therefore, we can say that since 2500 moles per second of carbon dioxide there the rate of enthalpy change will be here it will be there, what will be the rate of carbon dioxide production this is given 2500 moles per second of carbon dioxide. So we can say therefore, for 2500 moles per I think in second that is of carbon dioxide flow or production you can say the rate of enthalpy change will be it will be 2500 that is moles per second.

Whereas, this enthalpy change is given here -719. So into -719.5, this will be your you know kilojoule. So this is in terms of you know second. So here finally it will come as it will be here 1.80 into 10 to the power 6 kilojoule per second. So this is your you know final answer that how that you know enthalpy change that is specific enthalpy change for moles of carbon dioxide will be there.

And if that carbon dioxide production rate is 2500 moles per second then total amount of enthalpy change per second that will be is equal to 1.8 into 10 to the power 6 kilojoule per second. So in this way we can calculate that heat of reaction and then you know finally, at a certain rate what should be the you know enthalpy change there.

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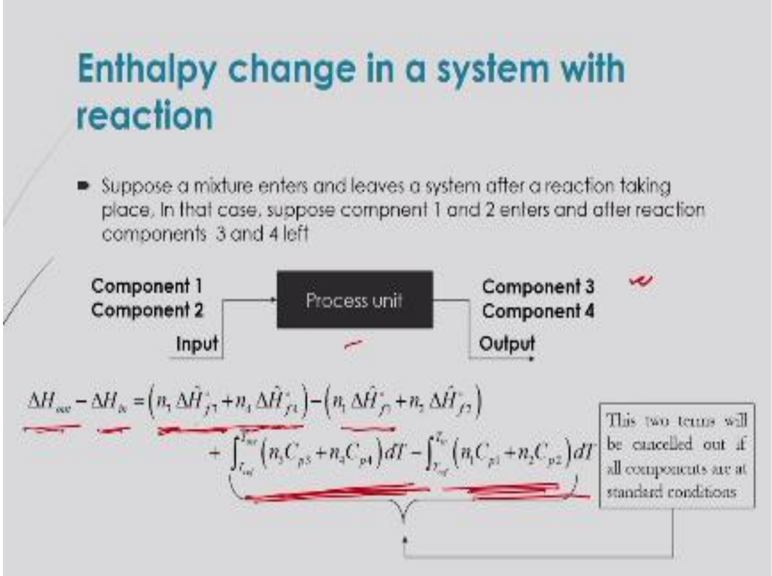

Enthalpy change in a system with reaction

- Suppose a mixture enters and leaves a system after a reaction taking place. In that case, suppose compnent 1 and 2 enters and after reaction components 3 and 4 left

$$\Delta H_{out} - \Delta H_{in} = \left(n_3 \Delta \hat{H}^{\circ}_{f3} + n_4 \Delta \hat{H}^{\circ}_{f4}\right) - \left(n_1 \Delta \hat{H}^{\circ}_{f1} + n_2 \Delta \hat{H}^{\circ}_{f2}\right) + \underbrace{\int_{T_{ref}}^{T_{out}} \left(n_3 C_{p3} + n_4 C_{p4}\right) dT - \int_{T_{ref}}^{T_{in}} \left(n_1 C_{p1} + n_2 C_{p2}\right) dT}$$

This two terms will be cancelled out if all components are at standard conditions

Now let us consider the system for enthalpy change you know for a mixture in a process unit. In that case suppose a mixture enters and leaves the system after a reaction taking place. So in that case, suppose component one and component two enters and after reaction components three and four are left there as per you know flow diagram given in this slide.

So here in this process unit, the component one and component two are coming as input in this process in unit and after reaction in this process unit, you will see that there will be some formation of components and you will see that components will be leaving from this process unit as component three and component four as output.

Now based on this you have to calculate what should be the enthalpy change from this inlet and outlet portion. So in that case you have to calculate what will be the enthalpy change in output and what will be the enthalpy change in the input. So thus delta H out minus delta H in that can be calculated based on that formation of that components in the inlet and outlet.

Now in this you know outlet condition what will be the components that is component three and component four and for that component three and component four what should be the enthalpy change. Now that enthalpy change can be calculated based on their you know heat of formation of that components.

Now heat of formation for this component three that is delta H f. Now in specific form that is delta H hat f 3 that is in zero that means in standard condition. So if you multiply it by n 3 that means here suppose moles of components three there is n 3.

Similarly, for component four similarly we can calculate it for that enthalpy change in that you know total enthalpy in the inlet condition as here delta H f 1and delta H f 2 and that can be actually obtained from that you know that heat of formation of that respective component one and two.

After that, you have to you know calculate that how that enthalpy change based on that operating condition. Now if your operating condition is not that of standard condition that is 25 degrees Celsius and one atmosphere, if it is changed at a certain temperature and pressure then you have to calculate that enthalpy change because of this temperature change.

So what is that enthalpy change or sensible heat change because of that temperature that you have to calculate form this equation here. Here basically you have to know that specific heat capacity for individual components in the inlet and outlet and what is the temperature difference from that the standard condition or difference from the reference condition up to that you know operating condition.

And then you have to integrate it based on this you know specific heat capacity if that specific heat capacity depends on the temperature. If it is constant then is not required to integrate here. Simply you have to multiply that specific capacity with the you know moles as well as the temperature difference.

Similarly, you have to calculate it for you know, reactant or input you know components and then output components along with that. So here these two terms will be cancelled out if all components are at a standard condition. That you have to remember that if you are considering only standard you know condition that means your reference temperature and then T out or you can say that T in that will be your reference.

So that is why here integration limit will be there at the same temperature. So here in this case this dT terms will be zero. So basically this sensible heat will be you know zero and this also will be zero. So accordingly we can say that at you know reference temperature or standard condition, standard temperature, this sensible heat terms will be cancelled out.

So other than this you know standard condition of course, you have to consider these two sensible heat. Again, there if there is a phase change during that temperature change, then you have to consider that enthalpy change during the phase change also.

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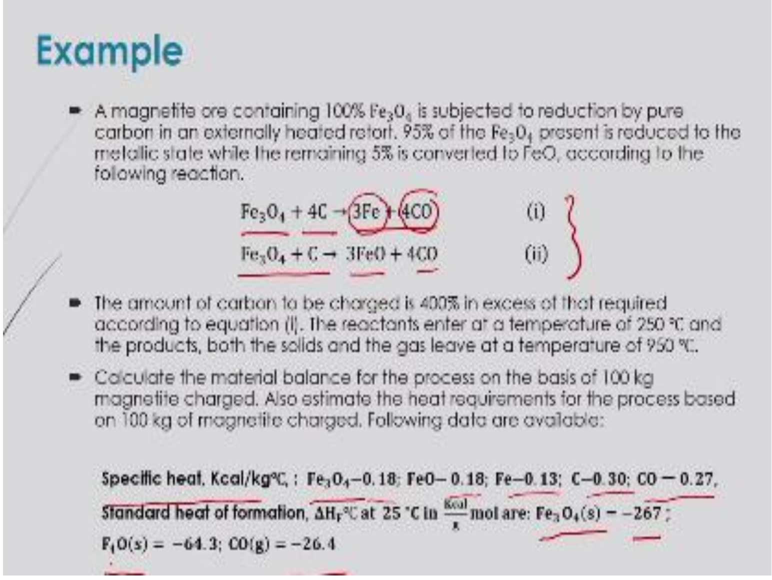

Example

- A magnetite ore containing 100% Fe_3O_4 is subjected to reduction by pure carbon in an externally heated retort. 95% of the Fe_3O_4 present is reduced to the metallic state while the remaining 5% is converted to FeO, according to the following reaction.

$$Fe_3O_4 + 4C \rightarrow 3Fe + 4CO \quad \text{(i)}$$

$$Fe_3O_4 + C \rightarrow 3FeO + 4CO \quad \text{(ii)}$$

- The amount of carbon to be charged is 400% in excess of that required according to equation (i). The reactants enter at a temperature of 250 °C and the products, both the solids and the gas leave at a temperature of 950 °C.
- Calculate the material balance for the process on the basis of 100 kg magnetite charged. Also estimate the heat requirements for the process based on 100 kg of magnetite charged. Following data are available:

Specific heat, Kcal/kg°C, : $Fe_3O_4 - 0.18$; $FeO - 0.18$; $Fe - 0.13$; $C - 0.30$; $CO - 0.27$,

Standard heat of formation, ΔH_F°C at 25 °C in $\frac{Kcal}{g}$ mol are: $Fe_3O_4(s) - -267$;

$F_eO(s) = -64.3$; $CO(g) = -26.4$

Now let us have an example for this you know theory here. Now in this case it is given that a you know magnetite ore you know that in different you know naturally occurring different you know compound conjugated in a particular you know soil form or stone form where it is called that you know ore and from where this ore after processing we can get different you know valuable mineral particles.

Now in this case this is a magnetite ore, that is one important ore from which you can you know separate that you know iron and from which we are getting different you know product of that iron. Now during that you know ore processing there, a magnetite ore that will contain you know 100% suppose Fe 3 O 4 now it is to be subjected to reduction by pure carbon in an externally heated you know, retort there.

So in that case this you know magnetic ore or magnetite ore is generally is bond with carbon at a certain temperature and then you will see that after bonding you will see that this you know this iron ore will be you know separated into a different products after reduction. And it is seen that 95% of that iron ore present in you know is reduced to the metallic state while the remaining that is 5% is converted into you know, ferrous oxide.

So according to that, according to this following equations given here as one and two in the slide, you see here that this iron ore Fe 3 O 4 with carbon, it will give you that metallic form of you know iron as and also you know that carbon monoxide. And again this you know ore also will give you that ferrous oxide and carbon monoxide there as equation number two.

Now the amount of carbon to be charged is 400% in excess of that required according to equation one. Now the reactants enters at a temperature of 200 degrees Celsius and the products both the solids and gas leave at a temperature of here 950 degree Celsius. Now calculate the material balance for the process on the basis of 100 kg magnetite that is charged into the you know retort.

Also have to estimate that heat requirements for the process based on 100 kg of magnetite ore that is charged. Now following datas are given to you like a specific heat capacity of that you know compound here, Fe 3 O 4 it is given as 0.18 and ferrous oxide it is given to you. Even iron it is given to you. Carbon it is given to you.

Carbon monoxide also it is given to you. So all are specific heat capacity. And similarly, standard heat of formation of all those compounds also given at standard condition that is at 25 degrees Celsius and for that for iron you know oxide that is ore the standard heat of formation it is given, -267 whereas ferrous oxide it is given is -64.3 and carbon monoxide it is given as -26.4.

We have to solve this problem to estimate the heat requirements for the process based on 100 kg of magnetite ore that is charged into the retort. What to do here, you have to write first what is the basis for this.

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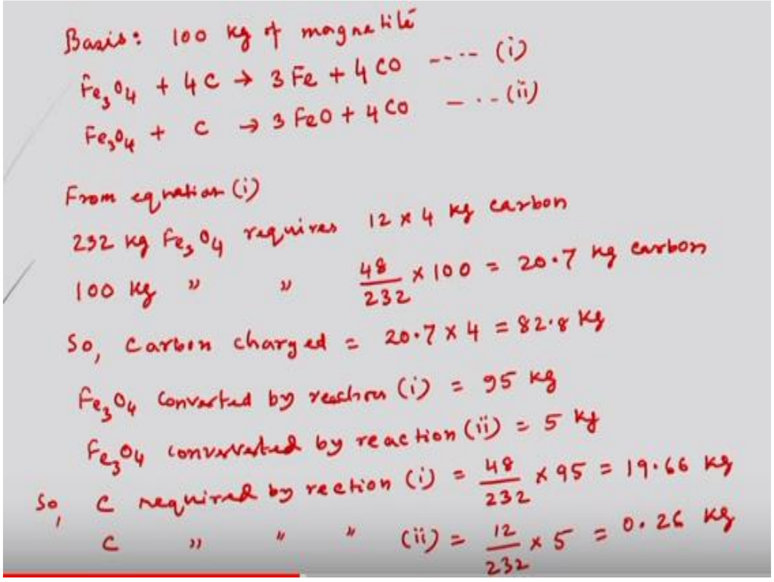

Basis: 100 kg of magnetite

$Fe_3O_4 + 4C \rightarrow 3Fe + 4CO$ ---- (i)

$Fe_3O_4 + C \rightarrow 3FeO + 4CO$ --- (ii)

From equation (i)

232 kg Fe_3O_4 requires 12×4 kg carbon

100 kg " " $\frac{48}{232} \times 100 = 20.7$ kg carbon

So, carbon charged = $20.7 \times 4 = 82.8$ kg

Fe_3O_4 converted by reaction (i) = 95 kg

Fe_3O_4 convervated by reaction (ii) = 5 kg

So, C required by reection (i) = $\frac{48}{232} \times 95 = 19.66$ kg

C " " " (ii) = $\frac{12}{232} \times 5 = 0.26$ kg

So the basis of this you know problem to be considered as know 100 kg of magnetite, and your reaction is Fe 3 O 4 plus 4 moles of carbon, which will give you the 3 moles of iron plus 4 moles of carbon monoxide as reaction one and the second reaction again it will be Fe 3 O 4 plus carbon one mole, which will give you the 3 moles of ferrous oxide plus 4 moles of carbon monoxide.

And here we can say that this equation, these two equations will be used to you know calculate first in terms of you know moles what is charged and what will be the most of that products are formed there. So from equation one, from equation one we can write 232 kg of Fe 3 O 4 requires 12 into 4 kg of carbon.

Why 12? 12 is the molecular weight of carbon and here since 4 moles of carbon is required, so here 4 into 12 kg of carbon is required. So here 232 is basically that molecular weight of this Fe 3 O 4. So we can say that, since 100 kg of this ore is charged, so 100 kg of Fe 3 O 4 requires then 48 divided by 232 into 100. That will be equals to 20.7.

This is you know kg of carbon. So this amount of carbon to be you know required to you know bond this you know 100 kg of iron ore there. So carbon charged will be equals to 20.7 into 4. That will be equals to here 82.8 kg. Now Fe 3 O 4 converted we know that by this reaction one, by this reaction one will be equal to 95 kg.

So Fe 3 O 4 converted by reaction two will be equals to 5 kg. So we can write here carbon required by reaction one. So carbon required by reaction one will be equal to 48 by 232 into here 95 kg. So it will be coming as 19.66 kg. Similarly, carbon required by reaction two that will be is equal to 12 by 232 into 5.

So it will be coming as 0.26 kg. So this amount of carbons are required for this respective reaction one and two. Then what will be the total carbon used.

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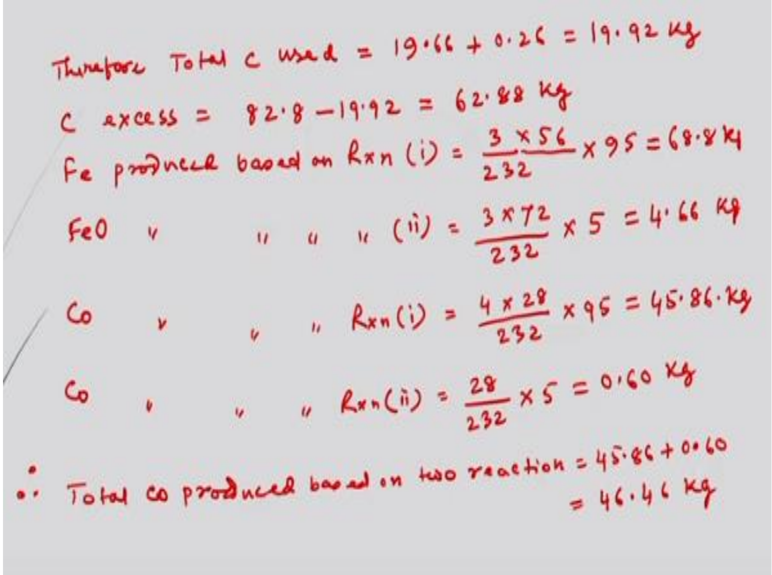

Therefore Total C used = 19.66 + 0.26 = 19.92 kg

C excess = 82.8 − 19.92 = 62.88 kg

Fe produced based on Rxn (i) = $\frac{3 \times 56}{232} \times 95 = 68.8$ kg

FeO " " " " (ii) = $\frac{3 \times 72}{232} \times 5 = 4.66$ kg

Co " " " Rxn (i) = $\frac{4 \times 28}{232} \times 95 = 45.86$ kg

Co " " " Rxn (ii) = $\frac{28}{232} \times 5 = 0.60$ kg

∴ Total co produced based on two reaction = 45.86 + 0.60
= 46.46 kg

Therefore, total carbon used in this two reactions that will be is equal to first one is 19.66, second one is 0.26 kg. So total it will be coming as 19.92 kg. And then carbon excess here, will be is equal to what is carbon supplied, what is the amount of carbon supplied? It is 82.8. Whereas, required amount is 19.92.

If you subtract this amount then you will get that carbon in excess. That will be is equal to here it will be coming as 62.88 kg. So this amount of carbon will be in excess in the retort. Now we have to find out what will be the iron is produced based on this reaction one and reaction two.

Iron produced based on reaction one, that will be is equal to, you know that 3 kg is produced out of 232 kg of that iron ore into here it will be 56. Here 3 into 56 means molecular weight of iron is 56, 3 to 56. This amount of you know iron will be produced out of 232 kg of you know magnetite ore that is you know as per reactions.

You have that you know total 95 kg of iron you know there. So it will be here iron oxide there. So total iron produced based on this 95 kg of magnetite ore, it will be here 68.8 kg. Similarly, iron produced based on reaction two it will be is equal to 3 into 72 divided by, this is iron oxide FeO, ferrous oxide is produced.

Based on reaction two it will be here 3 into 72 divided by 232 into what will be the amount of here you know, iron ore there in the reaction two this is 5. So it will be coming as 4.66 kg. And carbon monoxide produced based on reaction one that will be is equal to 4 into 28 divided by 232 into magnetite ore amount is 95 in reaction one.

So it will be coming as here 45.86 kg as per calculation. Similarly, we can say that carbon monoxide produced based on reaction two it will be here simply 28, since here is one mole. So this is 28 by 232. This is molecular weight of magnetite ore into what will be the amount of you know magnetite ore is taking part in that reaction two, it is 5 kg.

So total amount will be equals to 0.60 kg of carbon monoxide that is produced based on the reaction two. Therefore we can say that total carbon monoxide produced, total carbon monoxide produced based on two reactions that will be is equal to 45.86 + 0.60 that will be as 46.46 kg. So this amount of total carbon monoxide will be produced.

So we are getting different components that are produced based on that reaction as well as what are the you know that materials that is entering into the retort that is iron oxide ore or magnetite ore and carbon.

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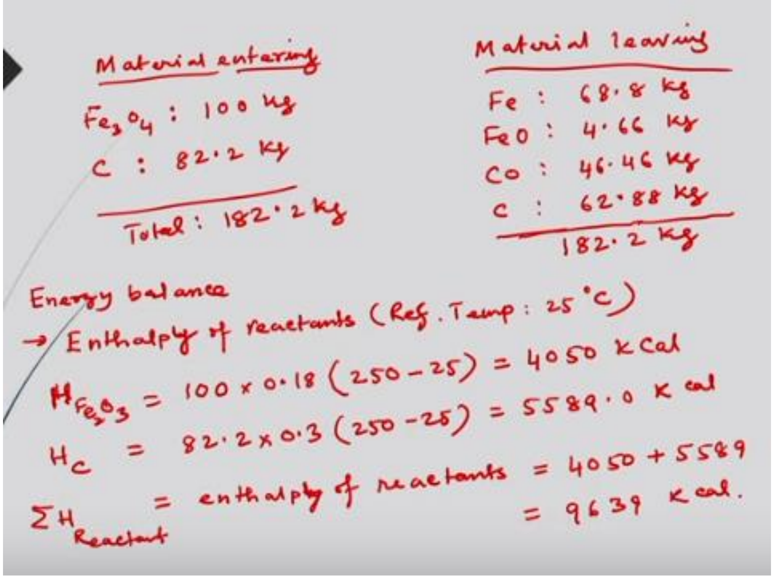

Material entering

Fe_3O_4 : 100 kg

C : 82.2 kg

Total : 182.2 kg

Material leaving

Fe : 68.8 kg

FeO : 4.66 kg

CO : 46.46 kg

C : 62.88 kg

182.2 kg

Energy balance

→ Enthalpy of reactants (Ref. Temp : 25 °C)

$$H_{Fe_2O_3} = 100 \times 0.18\,(250-25) = 4050 \text{ k Cal}$$

$$H_C = 82.2 \times 0.3\,(250-25) = 5589.0 \text{ k cal}$$

$$\Sigma H_{Reactant} = \text{enthalpy of reactants} = 4050 + 5589$$

$$= 9639 \text{ k cal.}$$

So we can summarized here as here material entering, and material leaving. So we can say here the material entering as Fe 3 O 4, this amount is 100 kg. Carbon, this amount is 82.2 kg. Then total 182.2 kg. Similarly, material leaving iron as a metal that is 68.8 kg. FeO that is ferrous oxide, it is 4.66 kg.

Carbon monoxide it is coming 46.46 kg. Similarly, carbon it is 62.88 kg. So here total amount that is leaving the retort it will be after summing up, it will be coming as 182.2 kg. So here we can say that as per material balance input and output will be same.

Whereas as output, we are getting different components based on that you know reaction conditions or reaction, you know component material balance. Next we have to do the energy balance. Now in this case you have to first consider that what will be the enthalpy of reactants at reference temperature.

So we say that here enthalpy of reactants reference temperature is 25 degree Celsius. Reference temperature is 25 degree Celsius based on which we can say enthalpy of this you know inlet condition delta H sorry H Fe 2 O 3 for this component. This will be is equal to this amount is 100 kg and specific heat capacity is given as 0.18.

And then temperature difference is here at 250 degrees Celsius this is burning reference temperature is 25 degrees Celsius. So this enthalpy for this you know magnetite ore at its you know inlet condition as a reactant, this will be coming as

4050 kilocalorie. Similarly, you have to calculate the enthalpy for carbon for the change of temperature of 250 degree Celsius from this reference temperature.

Whereas this carbon amount is given 82.2 kg at its inlet as a reactant. What is the specific heat capacity? It is given 0.3 and the temperature difference is 250 – 25. Then it will come as 5589.0 kilocalorie. So summation of this enthalpy for this reactant that will be is equal to you know enthalpy of reactants, it is called enthalpy of reactants.

So it will be equals to here 4050 + 5589. So total amount will be is equal to 9639 kilocalorie. So this is your total enthalpy in the reactant side. Now similarly you have to calculate what will be the enthalpy of product.

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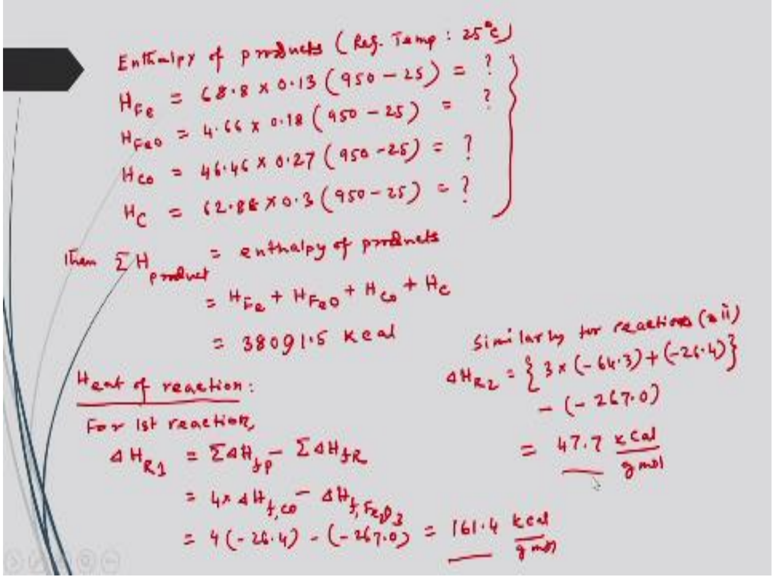

Enthalpy of products (Ref. Temp : 25°C)

$H_{Fe} = 68.8 \times 0.13\,(950 - 25) = ?$

$H_{FeO} = 4.66 \times 0.18\,(950 - 25) = ?$

$H_{CO} = 46.46 \times 0.27\,(950 - 25) = ?$

$H_{C} = 12.88 \times 0.3\,(950 - 25) = ?$

Then $\Sigma H_{product}$ = enthalpy of products

$= H_{Fe} + H_{FeO} + H_{CO} + H_{C}$

$= 38091.5$ kcal

Heat of reaction:

For 1st reaction,

$\Delta H_{R1} = \Sigma \Delta H_{fP} - \Sigma \Delta H_{fR}$

$= 4 \times \Delta H_{f,CO} - \Delta H_{f,Fe_2O_3}$

$= 4(-26.4) - (-267.0) = \underline{161.4}\ \frac{kcal}{gmol}$

Similarly for reaction (ii)

$\Delta H_{R2} = \{3 \times (-64.3) + (-26.4)\} - (-267.0)$

$= \underline{47.7}\ \frac{kcal}{gmol}$

So enthalpy of product. Enthalpy of products based on this reference temperature is 25 degrees Celsius. So you can say that here, product side as enthalpy of this iron metal that will be is equal to amount is 68.8 as per material balance into you know specific heat capacity is given 0.13.

And temperature difference is here at the outlet condition temperature is 950 degrees Celsius and the reference temperature is 25. So finally it is coming as you know some amount that is what is the amount that you can calculate it here. Similarly, H FeO you can get it 4 point similarly 66, into 0.18 specific heat capacity, the temperature difference again 950 - 25 here.

Similarly enthalpy for carbon monoxide, total amount of carbon monoxide is pound as per material balance is 46.46 kg into specific heat capacity is given 0.27 and the temperature difference is 950 – 25. So what will be the amount that you have to calculate.

What will be the, so enthalpy of remaining that carbon, which is not you know taking part in the reaction that is which is in excess that can be calculated as here, that amount is 62.88 kg. And specific heat capacity it is given 0.3 and the temperature here 950 minus reference temperature 25. Then what will be the amount.

Then total enthalpy of this you know product we can get here simply enthalpy of products that will be is equal to H Fe + H Fe 0 + H CO + H C. So it will be coming as total amount after substitution of all these values here it will be coming as 38091.5 kilocalorie. So this much of enthalpy will be for the total product components for the change of temperature.

Next, you have to calculate based on this what will be the heat of reaction. Heat of reaction we have to then calculate heat of reaction. Now for first reaction, for first reaction, we can say that delta H R 1, R for reaction, 1 for reaction one.

So this will be equal to summation of delta H f for product, f for formation p for product minus summation of delta H f for reactant here, here f for formation and R for here reactant. So it will be coming as 4 into delta H f of CO carbon monoxide, this is for product minus here delta H f, f for formation for Fe 2 O 3.

So this will be coming as 4 into -26.4. This is given to you minus -267.0. So finally it is coming as 161.4 kilocalorie per gram mole. Similarly, for reaction two. We can say delta H R 2 that will be is equal to 3 into -64.3 of this product iron oxide that is FeO plus -26.4 that is for carbon monoxide.

This one for product side minus reactant side there it will be you know minus of 267.0 this amount. So finally it is coming as you know 47.7 kilo calorie per gram mole. So heat of reaction for the first reaction it is coming 161.4. Whereas for second reaction it is coming here 47.7 kilocalorie per gram mole.

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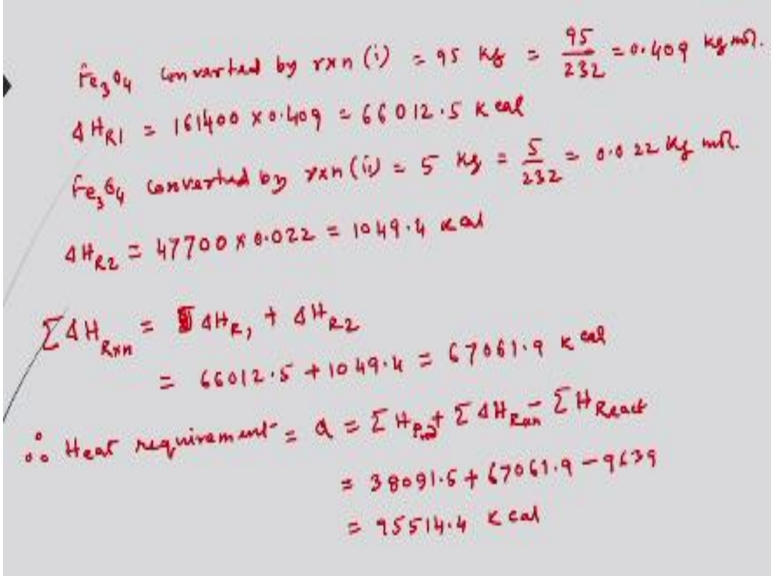

Fe_3O_4 converted by rxn (i) $= 95$ kg $= \frac{95}{232} = 0.409$ kg mol.

$\Delta H_{R1} = 161400 \times 0.409 = 66012.5$ kcal

Fe_3O_4 converted by rxn (ii) $= 5$ kg $= \frac{5}{232} = 0.022$ kg mol.

$\Delta H_{R2} = 47700 \times 0.022 = 1049.4$ kcal

$$\Sigma \Delta H_{Rxn} = \Delta H_{R1} + \Delta H_{R2}$$
$$= 66012.5 + 1049.4 = 67061.9 \text{ kcal}$$

$\therefore$ Heat requirement $= q = \Sigma H_{Prod} + \Sigma \Delta H_{Rxn} - \Sigma H_{React}$

$$= 38091.6 + 67061.9 - 9639$$
$$= 95514.4 \text{ kcal}$$

Since we can have this in terms of mole we can say that here Fe 3 O 4 converted by reaction one is equal to 95 kg this is basically 95 by 232. This is 0.409 kg mole. Similarly, we can say that for other components also and accordingly delta H that is enthalpy change for reaction one, it will be is equal to 161 point 161400.

Since it is you know kilocalorie per gram mole, so kg mole it will be here into here it will be 0.409. Then it is coming as 66012.5 kilocalorie. And Fe 3 O 4 here converted by reaction two that is amount is 5 kg. This is basically 5 by 232 kg mole. Then it will be 0.022 kg mole.

So enthalpy change for this reaction two that will be is equal to then if you multiply moles of this you know conversion of Fe 3 O 4 then it will come as here 47700 into 0.022 that will be 1049.4 kilocalorie. So total enthalpy change for these two reactions delta H Rxn that will be equal to or we can say summation of delta H R for reaction one and two.

So we can say that summation of you know delta H R 1 sorry this one plus enthalpy change for reaction two. So it will be coming as here as first one is 66012.5 plus for reaction two it is 1049.4. So total amount is coming as 67061.9 kilocalorie. Therefore, heat requirement as per problem, heat requirement that will be is equal to q.

This is basically summation of H p plus summation of delta H that is R minus summation of H reactant. This is reactant and this is product and this is heat of reaction. Now finally it will be coming as, what is that product side enthalpy, summation of that.

This is earlier we have calculated this is 38091.5 plus here heat of reaction is 67061.9 minus summation of enthalpy change because of that reactant components formation that is you know that 9639. So finally it is coming 95514.4 kilo calorie.

So this mass of heat is required to bond that magnetite ore to get that metallic iron along with other you know gaseous components. So in this way, we can do the material balance as well as energy balance to find out the materials required or materials supplied which are taking part to the reactions.

And based on that reaction you know enthalpy change we can have what will be the total heat is actually required for the complete combustion of that ore to find out this metallic form of that metals as per reaction.

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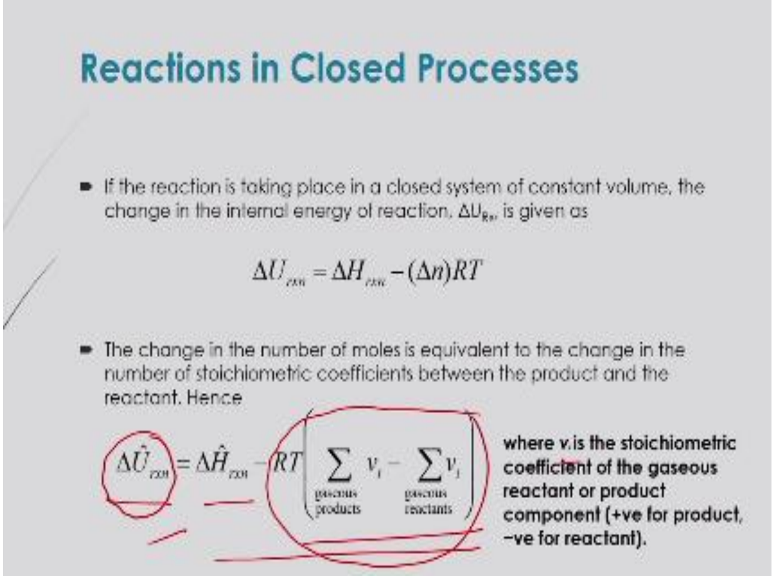

Reactions in Closed Processes

- If the reaction is taking place in a closed system of constant volume, the change in the internal energy of reaction, ΔU_{Rx}, is given as

$$\Delta U_{rxn} = \Delta H_{rxn} - (\Delta n)RT$$

- The change in the number of moles is equivalent to the change in the number of stoichiometric coefficients between the product and the reactant. Hence

$$\Delta \hat{U}_{rxn} = \Delta \hat{H}_{rxn} - RT\left(\sum_{\substack{\text{gaseous}\\ \text{products}}} v_i - \sum_{\substack{\text{gaseous}\\ \text{reactants}}} v_i\right)$$

where v_i is the stoichiometric coefficient of the gaseous reactant or product component (+ve for product, −ve for reactant).

Now these are all about that open process okay based on that reaction. Now suppose if reaction is going on in closed process and the reaction is taking place in a system where the volume will be kept constant and in that case the change in the internal energy of the reaction will happen and you have to find out that change of internal energy based on that reaction.

Now the change in that number of moles during that you know combustion of that, you know moles from its reactants to the product in that closed system, there are different components will be formed. Now the change of that you know reactant moles will be there.

And you will see that the change in that number of moles will be equivalent to the change in the number of stoichiometric coefficient between the product and the reactant. So in that case, we can write that what will be the internal energy change, because of that reaction in the specific terms like here specific heat of you know internal energy.

Then in that case that internal energy change will be is equal to what will be the enthalpy change for that reaction and in specific form. And then you have to you know calculate due to that temperature change and because of that you know closed system you will see that there will be a stoichiometric ratio changes because of that you know change of that you know pressure.

So based on which you can say total that you know that pressure and you know volume inside that reaction in the inside that you know closed system will be changing and that will change because of that you know what will be the you know stoichiometric coefficient of that product and stoichiometric coefficient of the you know reactants.

And based on which that net you know amount of moles change because of that reaction in the closed system. There will be a you know change of that you know pressure and volume because of that temperature change there. That can be calculated by this term here it is given.

So internal energy change can be calculated by this equation here based on that reaction where here you will see that this nu i is the stoichiometric efficient of the gaseous reactants or products components that is positive for the product and negative for the reactant to be considered.

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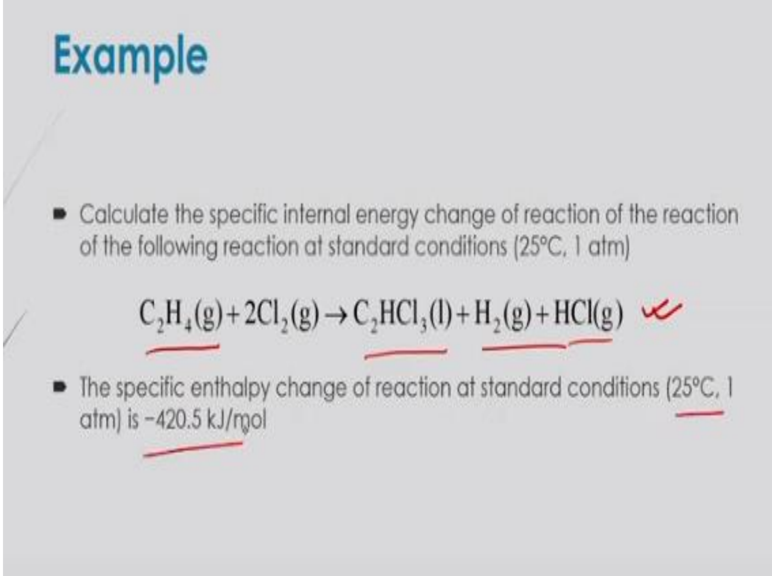

Example

- Calculate the specific internal energy change of reaction of the reaction of the following reaction at standard conditions (25°C, 1 atm)

$$\underline{C_2H_4(g)}+2Cl_2(g)\rightarrow \underline{C_2HCl_3(l)}+\underline{H_2(g)}+\underline{HCl(g)}$$

- The specific enthalpy change of reaction at standard conditions (25°C, 1 atm) is −420.5 kJ/mol

Now let us have an example here based on this concept. Now in this case you have to calculate the specific internal energy change of reaction of the following given at a standard conditions at 25 degrees Celsius and at one atmosphere. The reaction is here C 2 H 4 + 2Cl 2, which will give you that C 2 HCl 3 as a liquid and hydrogen and hydrogen chloride gas.

In this case the specific enthalpy change of reaction at standard conditions is 25 degrees Celsius and one atmosphere is given here -420.5 kilojoule per mole. Let us solve this problem here again based on that concept.

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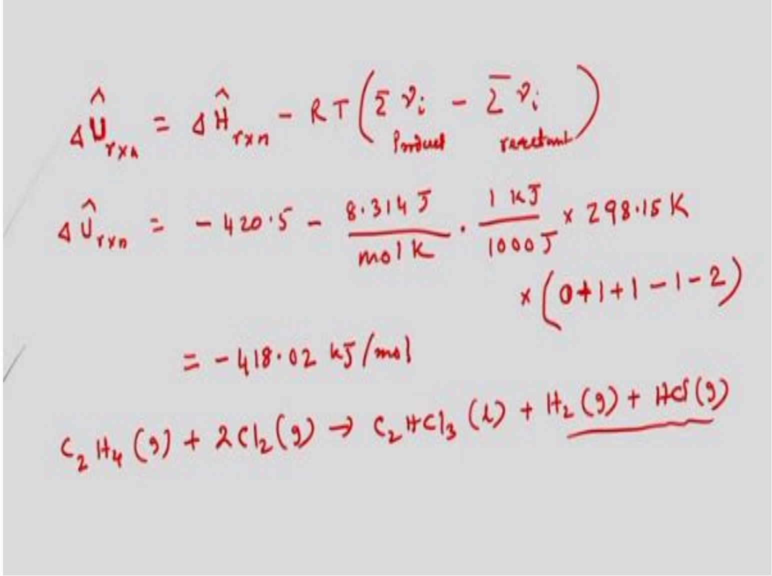

$$\Delta\hat{U}_{rxn} = \Delta\hat{H}_{rxn} - RT\left(\sum_{\text{Product}} \nu_i - \sum_{\text{reactant}} \nu_i\right)$$

$$\Delta\hat{U}_{rxn} = -420.5 - \frac{8.314\ J}{mol\ K}\cdot\frac{1\ kJ}{1000\ J}\times 298.15\ K \times (0+1+1-1-2)$$

$$= -418.02\ kJ/mol$$

$$C_2H_4(g) + 2Cl_2(g) \rightarrow C_2HCl_3(l) + \underline{H_2(g) + HCl(g)}$$

Now here apply this equation of internal energy change like delta U hat that is for you know reaction. This is basically enthalpy change, specific enthalpy change of reaction minus RT into summation of that is nu i for this you know product side component minus summation of nu i, this is for reactant side you know components.

So based on this equation, we can then write here delta U hat reaction that will be is equal to, it is given that enthalpy change for this minus 420.5 minus r, r value is 8.314 that is in joule by mole K into here you have to convert it to kilojoule. Here 1000 joule. This is basically one kilojoule.

Then temperature is here 298.15 Kelvin into here you know that product side stoichiometric ratio as per reaction, what is that reaction? Let us write this reaction here again. C 2 H 4 that is in gaseous form plus 2 Cl 2 that is chlorine gas in gaseous form. Here it will be forming as chloroform C 2 HCl 3 l and plus H 2 z and then hydrogen chloride in gaseous form.

Now here in this product side the stoichiometric is one plus one plus we can see that here we can write here 1 + 1 plus here what is that? We have not to consider that here the liquid form. So only 1 + 1 that is gaseous forms to be considered. And then, what will be the here we can say this is basically this is 0 + 1 + 1.

Then here minus and the product side it will be here C 2 H 4 it is one and then minus. It will be chlorine is I think 2. So finally, you will get this much and after simplification and calculation we can say that it will be -418.02 kilojoule per mole. So this is your internal energy change because of this reaction in a closed vessel where you will see only temperature can be changed.

But if it is you know that adiabatic you know chamber or closed vessel, there will be no change in temperature. So at constant temperature you have to consider that. If you are having that temperature change, then you have to consider also at what temperature you are going to calculate this internal energy change that temperature to be considered there.

I think we have done enough example for understanding the you know enthalpy balance or energy balance with you know heat of reaction calculation and also in open systems also if there are several you know components as a reactants and in the product side also there are several components as a product side components and how their enthalpy changing whenever temperature will be changing from its reference temperature.

So I think you understood this you know this energy balance with this reaction in open system and closed system. So in the next lecture we will try to discuss more about that energy balances of you know, heat of combustion. During that combustion how you can calculate that you know enthalpy change based on that product and you know reactant side components and their formation. So thank you for your giving attention.