# Fundamentals Of Combustion (Part 1)
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## Lecture – 13
## Adiabatic flame temperature

Let us start this lecture with a thought process “I would call him as a traitor who having educated at expense society not paying any heeds to the society”. Swami Vivekananda because I have chosen this thing because of 15th August was a independence day. So, and we should contribute for the society and to have a good bond with the society right and if you recall that in the last lecture we discussed about basically, how to calculate the heat of reaction using the bond energy and later on will look at thermo chemistry law that is known as Lavoisier, Laplace law and which helps on in basically using the heat of formation in the forward or the reverse directions right and now will be discussing about a Hess Law.

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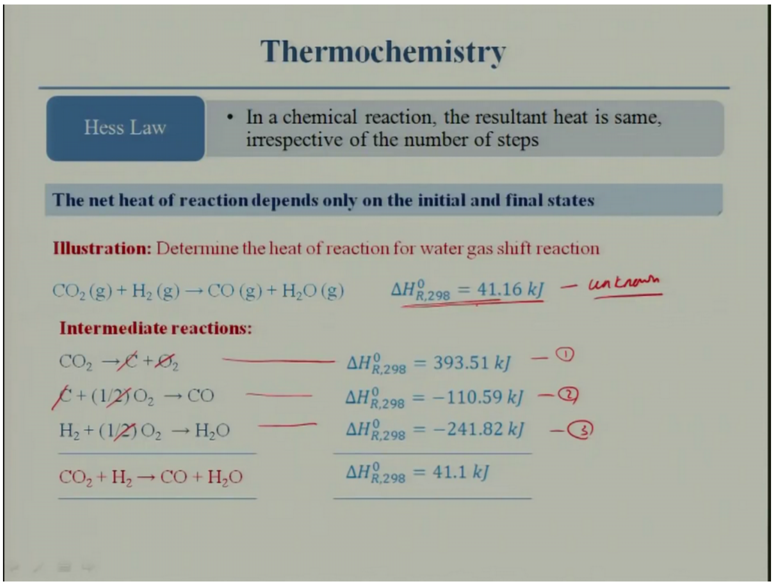

**Thermochemistry**

**Hess Law**

- In a chemical reaction, the resultant heat is same, irrespective of the number of steps

**The net heat of reaction depends only on the initial and final states**

**Illustration:** Determine the heat of reaction for water gas shift reaction

$CO_2\,(g) + H_2\,(g) \rightarrow CO\,(g) + H_2O\,(g)$ $\quad \underline{\Delta H^0_{R,298} = 41.16\ kJ}$ – unknown

**Intermediate reactions:**

$CO_2 \rightarrow \cancel{C} + \cancel{O}_2$ ——— $\Delta H^0_{R,298} = 393.51\ kJ$ – ①

$\cancel{C} + (1/\cancel{2})\,O_2 \rightarrow CO$ ——— $\Delta H^0_{R,298} = -110.59\ kJ$ – ②

$H_2 + (1/\cancel{2})\,O_2 \rightarrow H_2O$ ——— $\Delta H^0_{R,298} = -241.82\ kJ$ – ③

$CO_2 + H_2 \rightarrow CO + H_2O$ $\quad \Delta H^0_{R,298} = 41.1\ kJ$

Which state that in a chemical reaction the total amount of heat will be same, whether it is taking a single step or it is taking a multiple steps. In other words it does not depend upon number of steps whatever the amount of heat being released right; that means, what it indicates it indicates that it is a path function or a point function it is independent of number of step; that means, independent of.

Student: (Refer Time: 01:53)

Path right; that means, it is a point function right so, and this is nothing, but your what you call the first law of thermodynamics and in other words the Hess Law states that, the net heat of reaction depends only on the initial and final state as I told it is a basically point function.

So, let us take an example we are interested to find out heat of reaction for water gas shift reaction which is a very familiar reaction, which you people will be knowing that is carbon dioxide is reacting with the hydrogen getting into carbon monoxide and water right. Of course, here I have given the heat of reaction is 41.16 kilo joule right, but suppose it is not given right. We can apply the you know Hess Law to find out what will be heat reaction.

How we will going to do because we will have to see how this you know reaction is taking place. It can right this reaction can be decompose into various steps can be used to have this reactions and for which the heat of reaction will be known. Right for example, like if we know that CO 2 is you know converted into C plus O 2. Then we know the heat of reaction for that which is happens to be endothermic reaction and that is heat of reaction for this reaction you know is 393.51 kilo joule.

And the carbon react with half moles of oxygen going to the carbon monoxide for that you know heat will be elevated and this is heat of reaction is minus 110.59 kilo joules and this is known right and hydrogen can react with oxygen is going to the water. So, if you look at if I sum it up all this reaction because heat of reaction for all this three reaction, if I can say this is reaction one this is two and this three.

All reactions are known then what I will do I will just sum it up and if you look at this is cancel it out and this two are cancelled with this and this is nothing, but CO 2 plus hydrogen going to the product CO and water. And the total if I sum all this three together I will get 41.16 kilo joule right. Suppose, I it is not known unknown right then I can find out by this intervened reactions applying the Hess Law very easily and find out this right. Are you getting my point the application of Hess Law so and this as I told its nothing, but basically comes from the first law of thermo dynamics.

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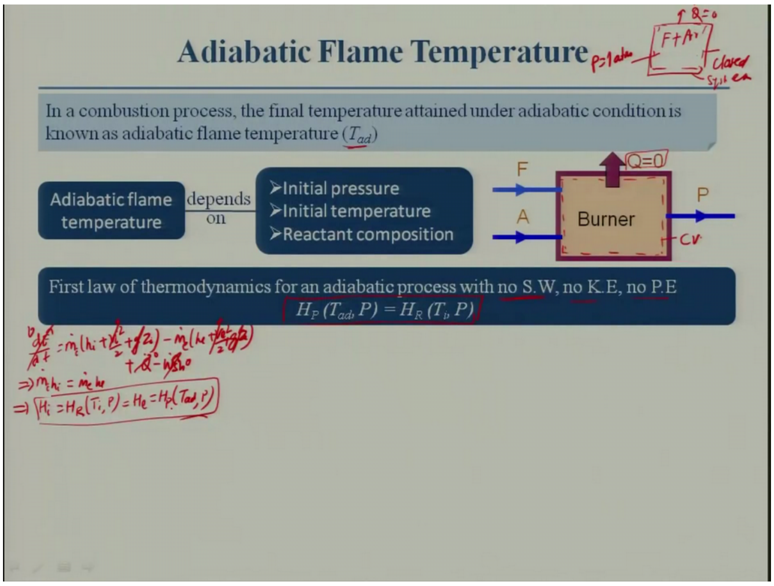

## Adiabatic Flame Temperature

In a combustion process, the final temperature attained under adiabatic condition is known as adiabatic flame temperature ($T_{ad}$)

Adiabatic flame temperature depends on

- Initial pressure
- Initial temperature
- Reactant composition

First law of thermodynamics for an adiabatic process with no S.W, no K.E, no P.E

$$\boxed{H_P(T_{ad}, P) = H_R(T_i, P)}$$

$$\cancelto{0}{\frac{dE}{dt}} = \dot{m}_i\left(h_i + \cancel{\frac{V_i^2}{2}} + \cancel{gz_i}\right) - \dot{m}_e\left(h_e + \cancel{\frac{V_e^2}{2}} + \cancel{gz_e}\right) + \cancelto{0}{\dot{Q}} - \cancelto{0}{\dot{W}_{sh}}$$

$$\Rightarrow \dot{m}_i h_i = \dot{m}_e h_e$$

$$\Rightarrow \boxed{H_i = H_R(T_i, P) = H_e = H_P(T_{ad}, P)}$$

Now, we will be using this thermo chemistry laws right for our calculations of heat of reaction heat of formations and other things right.

Now, having knowing how to handle this thing our main objective is to find out basically the flame temperature under adiabatic condition because that will tell us that how much maximum temperature one can get, if you are burning certain amount of fuel right. So, we will be now learning how to calculate that of course, you might have studied earlier also this thing, but let me repeat so, that you will be you know recall and then recapitulate it properly so, that you can use it.

In a combustion process if no heat is being transferred right which is not true because this under a vertical theoretical condition or a ideal condition where there would not be any heat transfer right.

And then you will attain a temperature which we call it as a adiabatic flame temperature right. This we call t adiabatic that is adiabatic temperature let us consider that you know one mole of fuel is getting into a burner along with certain amount of air and it is basically burning it and getting into a product right. For example, I can say that one mole of methane is reacting with two moles of air getting into one mole of carbon dioxide and two moles of water and what will be the product.

A nitrogen will be there right 3.74 into 2 moles of nitrogen right and if I will now I want to find out what will be the temperature at the exit of this burner right, provided no heat being transfer; that means, Q is equal to 0 right. Now, what we will do we will have to take a control volume right let us say this is our control volume right and keep in mind that this is a flow system right..

If it is a flow system then we will have to also make certain assumptions. What are those assumptions? Steady flow process then what else change in kinetic energy.

Student: (Refer Time: 07:49).

Will be 0, change in potential energy will be 0 right. Is there any work done here? The work done also is 0 right under these conditions you can invoke the first law of thermodynamics and then you will get that right.

Now, if you look at this adiabatic temperature will be depends on what, suppose you will get some temperature we can we will do that little later on, but it will be depend on what it will be depend on the what is the composition of the fuel air right or fuel oxidised right and it will be depend on the initial temperature or the initial pressure right. In this case suppose it is one atmospheric pressure right and if the reaction is taking place in this burner what will happen to the pressure?.

Student: (Refer Time: 08:48).

Will it increase? Certainly no right because it is a flow process right. So, therefore, it would not increase, but if this is not a flow process, but a closed chamber; let us say this is a chamber right is a closed chamber I am reacting with basically fuel plus air right. No heat is going out right this is my system and starting with initial pressure is one atmospheric pressure right one atmospheric pressure. What will happen to pressure? Pressure will increase because why temperature has increase and this is a control volume right. It is not a control volume; it is basically control mass system or a close system right close system. So, therefore, the pressure in this case pressure would not increase is that clear or not?

Now, from the first law of thermodynamics for a adiabatic process with no change in kinetic energy right, no change in potential energy there is no shaft work. I will get H P is equal to H R. Is it true? How I will get this? What is the meaning of H P is equal to H R? That means, enthalpy of the product is equal to enthalpy of the reactant how did I get this any idea.

Student: (Refer Time: 10:45).

That means.

Student: Will be absorbed by the (Refer Time: 10:49).

Product that is the meaning, but how did I arrive at this expression that is the question.

Student: (Refer Time: 10:55).

First so that means, you will have to write down your first law of thermodynamics right. What is that? That is d E by d t is equal to m dot I h i plus v i square plus g z i minus m dot e is the exit you can say h e plus v e square by g z e plus minus shaft work right steady it is 0 shaft work is 0. This potential energy is 0 right and adiabatic so, therefore, this is 0. So, therefore, what you will be getting you will be getting m dot i h i is equal to m dot e h e and in our example this is your reactant right m dot h i is nothing, but h i is equal to h reactant right. Yes or no? Which is basically t i it depend up on pressure, is equal to m dot e h e is nothing, but what h e is nothing, but your product which is adiabatic and pressure right are you getting its very simple right.

So, but what is this h r and h p basically we are doing enthalpy balance you know enthalpy of the reactant; total enthalpy of the reactant is same as the total enthalpy of the product. That is the point we are doing and then let me erase this portion.

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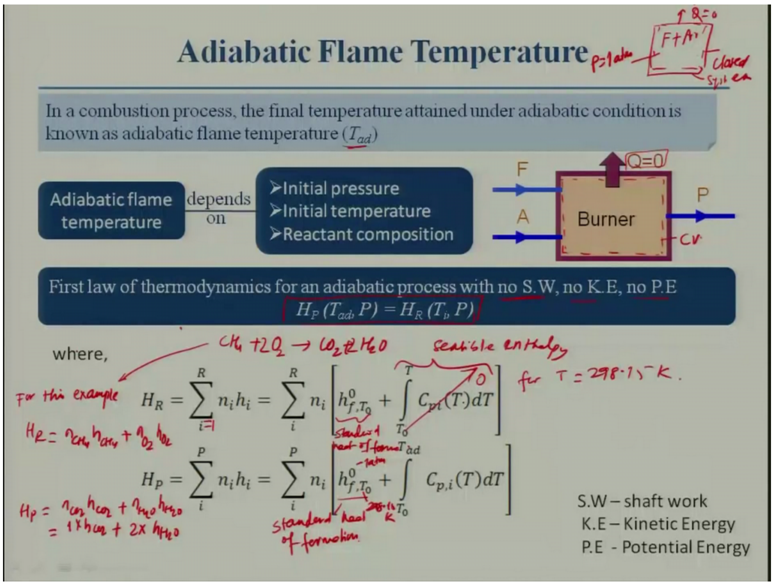

## Adiabatic Flame Temperature

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Adiabatic flame temperature depends on
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First law of thermodynamics for an adiabatic process with no S.W, no K.E, no P.E

$$H_P(T_{ad}, P) = H_R(T_i, P)$$

where,

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ sensible enthalpy

$$H_R = \sum_{i=1}^{R} n_i h_i = \sum_{i}^{R} n_i \left[ \underbrace{h^0_{f,T_0}}_{\text{standard heat of formation}} + \overbrace{\int_{T_0}^{T} C_{pi}(T)\,dT}^{0} \right]$$ for $T = 298.15$ K.

For this example

$H_R = n_{CH_4} h_{CH_4} + n_{O_2} h_{O_2}$

$$H_P = \sum_{i}^{P} n_i h_i = \sum_{i}^{P} n_i \left[ \underbrace{h^0_{f,T_0}}_{\text{standard heat of formation}} + \int_{T_0 \text{ } 298.15\text{ K}}^{T_{ad}} C_{p,i}(T)\,dT \right]$$

-1atm

$H_P = n_{CO_2} h_{CO_2} + n_{H_2O} h_{H_2O}$
$= 1 \times h_{CO_2} + 2 \times h_{H_2O}$

S.W – shaft work
K.E – Kinetic Energy
P.E - Potential Energy

Where H R is basically n i h i, i is the can be you know like 1 to R, 1 to R means what like if it is methane right if I am saying this is methane plus oxygen right going to the carbon dioxide water right. What will be mole n i for this? For the reactant side this reactant. Reactant means two reactant, one is methane other is your oxygen right. So, if I want to write down here H R, What value this one? n C H 4 h C H 4 0 or I will put naught, I would not put naught why because this is not only heat of formation. It is, will it be heat of formation? Yes it will be heat of formation, total heat formation right and then n o 2 h o 2 and this each heat of formation will be having two components one is.

Student: (Refer Time: 14:28).

This is standard heat of formation and this portion is sensible enthalpy right are you getting. For this example, for this example similarly I will have to look at the h product. In this case, in this example what will be H P, n C O 2, h C O 2 plus n water and h water. In this case n water will be two mole and n carbon dioxide will be one. Isn't it? Yes or no? Are you getting? This I can write down 1, this is 1 into h C O 2 plus 2 into h water and each will be having what you call again the heat of standard heat of formation right..

This is standard heat of formation why standard because it is at 298.15 Kelvin right t 0 and this 0 corresponding to 1 atmospheric pressure right and this t 0 is 298.15 Kelvin and this is form this is sensible enthalpy t 0 to t adiabatic and C p i keep in mind that specific heat is a function of temperature right. You will have to integrate over the you know t 0 to t adiabatic; that means, and this C p i is i means particular species; that means, C p will be dependent on temperature also the pertaining species right. So, how we will do that that is a big problem like you know how to calculate that and now so, if you want to use this then only you can calculate what it would be the adiabatic temperature and keep in mind that for the reactant it is t 0 to t. It happens to be the reactant at 298 Kelvin, What will happen? This will be 0 this will be 0 for t is equal to 298.15 Kelvin. If initial temperature is that, but if initial temperature is 600.

Student: 600

Kelvin then I cannot make it 0. The sensible enthalpy cannot be 0, it will be some finite value that will have to calculate is that clear. Now, what is here happening of course, this is we have looked at mathematically, but now we will be discussing little bit about you know the physically what is happening. What is happening can anybody tell me? Heat being release, if heat being release right those heat will be utilised to,.

Student: (Refer Time: 18:04).

Enhance the temperature of the product to certain values right and that we call it as a adiabatic temperature, provided no heat being transfer from system to a surrounding provided otherwise, will be lower than that lower than the adiabatic temperature. What we will get? If there is a heat transfer between system and surrounding ok is that clear?

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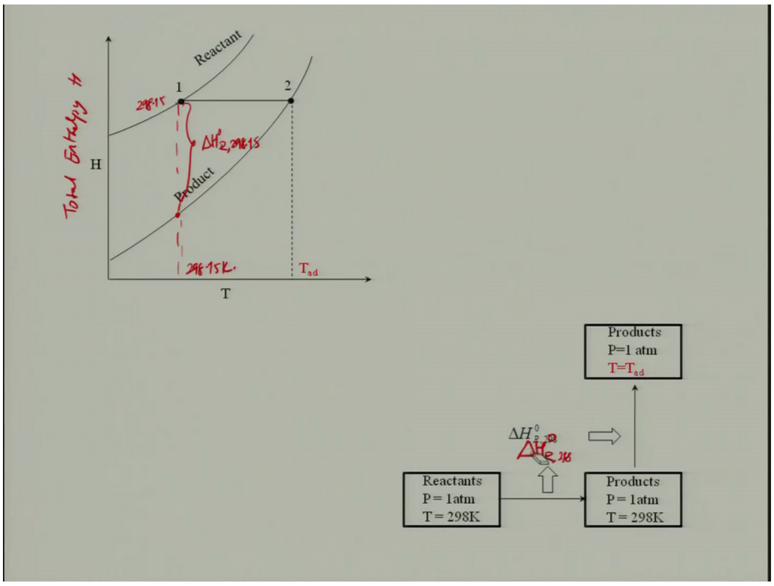

Products
P=1 atm
$T=T_{ad}$

Reactants
P = 1atm
T = 298K

Products
P = 1atm
T = 298K

Now, if you look at this is basically you know enthalpy line for the reactant, enthalpy line for the product with respect to temperature. This is your enthalpy total enthalpy right. Now if you recall that I had made these two parallel lines do you remember right, but now it is not parallel. Is it looks to be parallel? Right now this is basically if I say this happens to be 298.15 right this temperature of course, it is not possible this scale is not that I have just you know made like that otherwise it will be far away right and if you take a linear scale ok.

Now, if I say this thing what will be my this point here? This is basically 298.15 Kelvin. What would be this? This is what I will call?

Student: (Refer Time: 19:40).

No. This is heat of reaction right 298 let me right down 1.5, this amount of heat because that is corresponding to standard pressure and temperature right and this heat will be utilised to bring this product to adiabatic temperature. So, more pictorially if you want to say; that means, reactant has one atmospheric pressure 298.15 Kelvin. It is going to the product and this is the heat of reaction, right 0 right and then this heat will be utilised to take this product into T adiabatic. This is just to explain you, but in actual situation is it happening no and just to explain I am telling you actually it will be going on is that clear.

Now, suppose this we are doing right and this is a system right a control volume or an open system we have consider. Now, let us stay in a chamber we are what you call reacting let us say methane is a is reacting with oxidizer and getting into carbon dioxide and water. What will be the adiabatic temperature? How we will handle? Will it handle this way or we will have to do something? That is a question I am asking you please think about.

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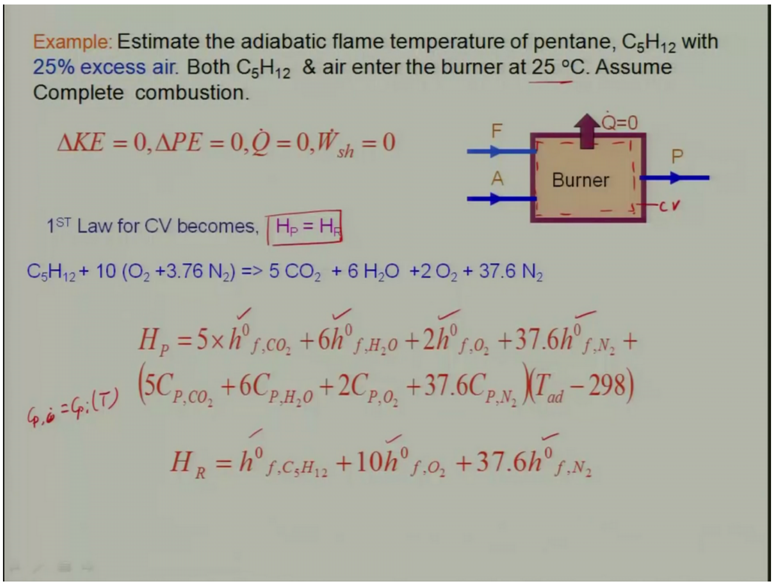

Example: Estimate the adiabatic flame temperature of pentane, $C_5H_{12}$ with 25% excess air. Both $C_5H_{12}$ & air enter the burner at 25 °C. Assume Complete combustion.

$$\Delta KE = 0, \Delta PE = 0, \dot{Q} = 0, \dot{W}_{sh} = 0$$

1ST Law for CV becomes, $\boxed{H_P = H_R}$

$C_5H_{12} + 10\,(O_2 + 3.76\,N_2) \Rightarrow 5\,CO_2 + 6\,H_2O + 2\,O_2 + 37.6\,N_2$

$$H_P = 5 \times h^0{}_{f,CO_2} + 6h^0{}_{f,H_2O} + 2h^0{}_{f,O_2} + 37.6h^0{}_{f,N_2} +$$

$$C_{p,i} = C_{p,i}(T) \quad \left(5C_{P,CO_2} + 6C_{P,H_2O} + 2C_{P,O_2} + 37.6C_{P,N_2}\right)\left(T_{ad} - 298\right)$$

$$H_R = h^0{}_{f,C_5H_{12}} + 10h^0{}_{f,O_2} + 37.6h^0{}_{f,N_2}$$

Now, we will take an example right to estimate the flame temperature of pentane C 5 H 12 right with a 25 percent excess air. Both pentane and air enter the burner at 25 degree celsius right. When we are talking about a burner, basically what is that meaning? Meaning is that we will be using an open system, it is a burner flow is taking place. So, therefore, an open system is a obvious choice and assume that complete combustion mean taking place; that means, what it will be having carbon dioxide and water and of course, it with air. So, therefore, nitrogen will be there it would not it is an inert gas for this example and of course, 25 percent excess air there; that means, some oxygen will be there at the end of combustion.

So, as I told I do will take an open system here right because is a burner control volume so, the same assumption will be doing change in kinetic energy is equal to 0, change in potential energy is 0, heat will be 0 and work done will be 0 right. This dot I am saying because it will be basically per second kind of thing you can say and first law of thermodynamics for control volume is nothing, but your H P is equal to H R right. Product total enthalpy of product is equal to total enthalpy of reactant (Refer Time: 23:08).

And this reaction we can consider that is basically pentane 1 mole of pentane is reacting with basically 10 moles of oxygen and you know nitrogen's and 5 moles of carbon dioxide, 6 moles of water and 2 moles of oxygen and 37.6 nitrogen. So, this is balanced of course, you will have to make you know I have just return down here, but you will have to balance right. Now, by from this you basically know the products right, product are known reactant anyway it has to be given to find out this thing.

Now, what you will do will say that and keep in mind that it is 25 degrees Celsius and we will have to find out H P, H P. What is your H P? H P is nothing, but 5 into heat of formation of carbon dioxide into 6 moles of water heat of formation of water plus 2 moles of oxygen and 37.6 of heat of formation and this is if you look at coming from the sensible enthalpy and T adiabatic minus 298 multiplied by the all this C P of, you know carbon dioxide, water oxygen and nitrogen and their respective mole moles right for the balance equation right this we know.

Now, in these thing interestingly these are all known you can find out these values from the table right. Total enthalpy of the reactant is basically summation of heat of formation to all the participating species like 1 mole of pentane and 10 moles of basically oxygen and 37 moles of nitrogen and you will have to substitute these values from the table right; that means, all are known you will have to just calculate right.

Now, question arises what the C P value I will be taking because C P is a function of temperature. Yes or no? C P is a function of,

Student: (Refer Time: 25:45).

Right C P is a function of temperature. What temperature I should take? Because I do not know the adiabatic temperature, if I know the adiabatic temperature there then I can very happily use that ok.

Now, let us do something we can do it iteratively right because I will give some values and then I will find out what it would be.

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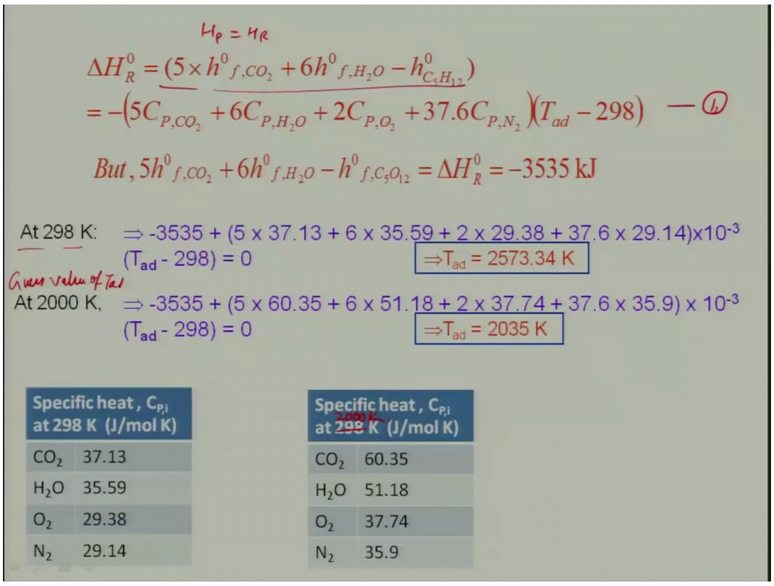

$H_P = H_R$

$$\Delta H_R^0 = \underbrace{(5\times} h^0{}_{f,CO_2} \underbrace{+6h^0{}_{f,H_2O} - h^0_{C_5H_{12}}})$$

$$= -\left(5C_{P,CO_2} + 6C_{P,H_2O} + 2C_{P,O_2} + 37.6C_{P,N_2}\right)\left(T_{ad} - 298\right) \quad — ①$$

$$But, 5h^0{}_{f,CO_2} + 6h^0{}_{f,H_2O} - h^0{}_{f,C_5O_{12}} = \Delta H_R^0 = -3535\ \text{kJ}$$

At 298 K: $\Rightarrow -3535 + (5 \times 37.13 + 6 \times 35.59 + 2 \times 29.38 + 37.6 \times 29.14)\times 10^{-3}$ $(T_{ad} - 298) = 0$ $\boxed{\Rightarrow T_{ad} = 2573.34\ K}$

Guess value of Tad

At 2000 K, $\Rightarrow -3535 + (5 \times 60.35 + 6 \times 51.18 + 2 \times 37.74 + 37.6 \times 35.9) \times 10^{-3}$ $(T_{ad} - 298) = 0$ $\boxed{\Rightarrow T_{ad} = 2035\ K}$

| Specific heat, $C_{P,i}$ at 298 K (J/mol K) | |
|---|---|
| $CO_2$ | 37.13 |
| $H_2O$ | 35.59 |
| $O_2$ | 29.38 |
| $N_2$ | 29.14 |

| Specific heat, $C_{P,i}$ at ~~298~~ 2000 K K (J/mol K) | |
|---|---|
| $CO_2$ | 60.35 |
| $H_2O$ | 51.18 |
| $O_2$ | 37.74 |
| $N_2$ | 35.9 |

If I substitute this H P is equal to H R and then I will find out this is nothing, but you heat of heat of reaction because this all are (Refer Time: 26:35). So, that you will get the heat of reaction, this you get from a table or you know this individual heat of formation of a individual species. Then you can calculate right and that happens to be 3535 kilo joule right.

Even you substitute these values from the table or from heat of reaction you can take from the table whichever is convenient, that will be 3535 kilo joules and what I will do? I will have to find a let us say that 298 Kelvin it would be it may not be, but I a am having too interest to hear to consider 298 Kelvin balanced right. Then what I will be I will be getting specific heat values for this various species as 298 Kelvin. These are the values right, 37.13 for carbon dioxide, water 35.59, oxygen 29.38, nitrogen 29.14..

So, if I substitute this values right all those here is right this expression right. This expression equation one you can say then I will get a temperature something 2573.34 Kelvin right. I am assuming this temperature is what the product temperature because these are all product, which one you these are all product. Carbon dioxide, water, oxygen, nitrogen are the product and that is a quite a big values right.

Now, I will take another guess that is 2000 Kelvin right it may be may not be right, but I will take that then I will get you know values substitute this values because these are the table. When sorry this will be 2000 Kelvin right and these are different you can compare with this C O 2 is very high because 37.13 and 60.35 is lot of because it is a triatomic molecule. Therefore, it is higher right and water of course, is higher, but not that much and oxygen and nitrogen there is also little bit higher, you substitute these values then what you will do you will get T adiabatic, 2035 Kelvin right..

Now, it is very closer you can do otherwise you can make a linear interpolation if it is a this temperature and nearby let us say 298 Kelvin and 2000 Kelvin you cannot do a linear interpolation. If it is let us say 1800 Kelvin, you have guess and 2000 it is a there is a difference and one is higher one is lower, you can do that linear interpolation. If it is interval is small and then you do let us say you are not happy with this thing 2035 Kelvin, you have guess 2000 right this is a guess right guess, value guess value of temperature T adiabatic right.

And then you are not happy then what you will do you take 2000, 2035 again after that and calculate and then you if you are not getting the matching properly. Then you take a linear interpolation calculate easily so, that is one way of doing ok.

This we will stop over, but you think about like the products is an unknown right and unless you choose the proper specific heat values, then you will land in a temperature which is quite different than that of the adiabatic temperature. So, with this will stop over and we will see in the next class about more about how to handle this chemical equilibrium and other things ok.

Thank you.