Fundamentals of Aerospace Propulsion
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Lecture – 18

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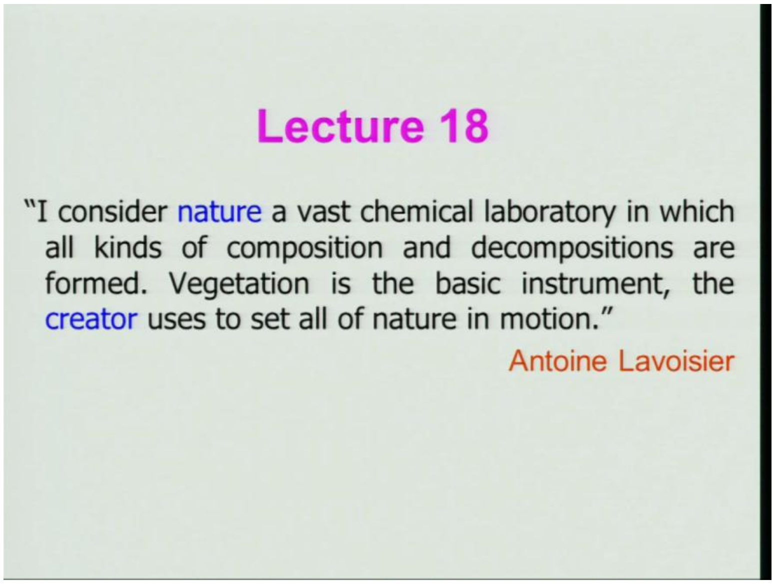

Lecture 18

"I consider nature a vast chemical laboratory in which all kinds of composition and decompositions are formed. Vegetation is the basic instrument, the creator uses to set all of nature in motion."

Antoine Lavoisier

Today, we will be talking about this thermodynamic of combustion, and with a thought passes from Lavoisier who says that I consider nature a vast is chemical laboratory in which all kinds of composition and decomposition are formed. Vegetation is the basic instrument the creator uses to set all the nature in motion. This is the very important, and the profound statement which you know our ancestors were very much aware that is why we were agricultural based country, and chemical reaction always takes place. And whatever the chemical reaction takes place in nature those are profound and without any effect that is very important point when we talk about chemical reaction will be talking about that. And as we discussed in the last lecture about the various you know like heat of formation, heat of reaction, heat of combustion and other thing how to calculate.

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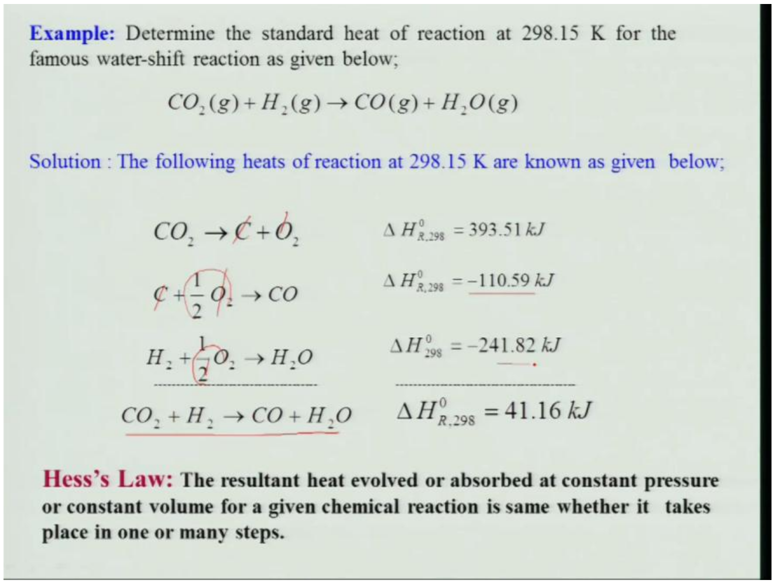

Example: Determine the standard heat of reaction at 298.15 K for the famous water-shift reaction as given below;

$$CO_2(g) + H_2(g) \rightarrow CO(g) + H_2O(g)$$

Solution : The following heats of reaction at 298.15 K are known as given below;

$CO_2 \rightarrow \cancel{C} + \cancel{O_2}$	$\Delta H^0_{R,298} = 393.51\ kJ$
$\cancel{C} + \frac{1}{2}\cancel{O_2} \rightarrow CO$	$\Delta H^0_{R,298} = -110.59\ kJ$
$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$	$\Delta H^0_{298} = -241.82\ kJ$
$CO_2 + H_2 \rightarrow CO + H_2O$	$\Delta H^0_{R,298} = 41.16\ kJ$

Hess's Law: The resultant heat evolved or absorbed at constant pressure or constant volume for a given chemical reaction is same whether it takes place in one or many steps.

Today what will do like, we will be looking at you know just to take an example about that and see how we can use. For example, like determine the standard heat of reaction at 298.15 Kelvin for famous water-shift reaction as given below. You know this is a very important water-shift reaction which is basically one mole of carbon dioxide reacting with hydrogen, it is going to the carbon monoxide and water. Of course, keep in mind that all the components are in gaseous state. Now question arises whereas I can get back you know carbon monoxide can be reacted with the oxidizer to give me what, carbon dioxide, am I right. If you look at like nature walks in cycle whether I can use this as a cycle or not; of course that is not the with this example, because we are interested to determine the standard heat of reaction at 298.15 Kelvin. And this is quite famous, you must be aware about this reaction that is water-shift reaction.

How to go about it I do not know this heat of reaction of this, you know of this particular reaction. Then what I will have to do, but however I will be knowing several other reaction. If I know those reaction can I really get this reaction heat of reaction; that means heat of reaction of these water-shift reaction can I get. Now, let us look at how we can get that is the following heat of reaction at 298 are known like for example like CO 2 is going to the C plus O 2. We know that, we also similarly know C plus half O 2 going to the CO. The carbon is reacting with oxygen to the CO and we know that hydrogen reacting with oxygen half I am going to water.

If I know this three reaction, you know if you add all this thing can I get this water-shift reaction yes or no? If you look at I can cancel this out and this oxygen, you know like about this half and half, this I can a cancel, what I land it CO 2 plus hydrogen, it going to the CO plus water right. I must knows this like heat of reaction heat of reaction for this CO 2 and C plus O 2 is basically 393.51 closure, of course that is 298.15 Kelvin.

Similarly, I know this reaction and keep in mind that the earlier reaction was positive, and this is negative that means the earlier reaction was endothermic, and this is exothermic reaction. And similarly, the heat of reaction for the third reaction that is hydrogen plus oxygen going to water is again an exothermic reaction. So if I just add this together as I told you earlier that what I will get, I will get CO 2 plus hydrogen going to the product CO and water. And if I add together, I will get this you know total heat of reaction for this reaction is equal to 41.16 kilojoules, just I will add all these three together. But what is the basis for it from where how can you do that is it right or wrong, can anybody tell me? That is basically known as Hess's law.

He states that resultant heat evolved or absorbed at constant pressure or a constant volume for a given chemical reaction is same weather it takes place in one or many steps. By the way this Hess's law come from where, from which law, but this is not really the actual law but people call it. It has come from your first law of thermodynamics, and this is a beautiful concept which is being you know as a Hess's law, which is just extension of the first law of thermodynamics. Whatever the path it takes, you know as long as it is having two ends point you know, then it will be dependent on the n point that means it is independent of path taken by the reaction.

So that is the basis of the first law of thermodynamics. If you remember like we are talking about internal energy property of this system. So and this is the one now what we will do, we have now worked with this heat of formation, heat of reaction then you know like how to get a heat of reaction by knowing the elementary reaction like CO plus half CO 2, CO kind of things. Now, how I will do all these things, what for we will do. Of course, you can say that I need to calculate or estimate the heat of combustion that is why I need this information. Keep in mind that heat of formation status are available in the table, tabulator form like Jan-up of table. Of course, in my book fundamental combustion, it is given on the backside in the appendix you can use those data.

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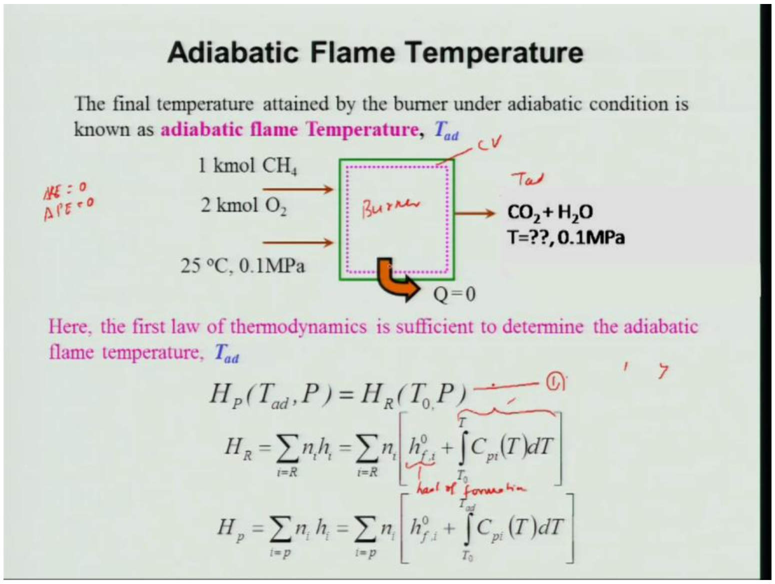

Adiabatic Flame Temperature

The final temperature attained by the burner under adiabatic condition is known as **adiabatic flame Temperature**, T_{ad}

Here, the first law of thermodynamics is sufficient to determine the adiabatic flame temperature, T_{ad}

$$H_P(T_{ad}, P) = H_R(T_0, P) \text{ ——— } ①$$

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

$$H_p = \sum_{i=p} n_i h_i = \sum_{i=p} n_i \left[h^0_{f,i} + \int_{T_0}^{T_{ad}} C_{pi}(T)\,dT \right]$$

Now, question there is there apart from estimating the heat of reaction or the heat of combustion whether we can use, those data for something else, can anybody tell me how we can use those data, which is essential when we talk about combustion. See we need to find out what will be the maximum temperature one we can think of that is the called it as an adiabatic flame temperature; that is the final temperature attained by the burner under adiabatic condition is known as adiabatic flame temperature. It can be burner like for example, we have taken a burner in which 1 kilo mole of methane is entering into the burner where it is reacting with 2 kilo moles of oxidizer, of course all these reactant that is methane and oxygen are add 25 degree Celsius and 0.1 megapascal.

Now if you look at that it is going to a product this CO 2 and water. And what will be the temperature here at the product. Of course, it may be at a pressure of 0.1 megapascal, and keep in mind that if I take this as my burner, this is my burner, what will be it is, it is basically I can take this as a control volume, this is my control volume. And no heat is going out of this burner, and what are the assumption we need to make, we will have to say that is the steady passes change in kinetic energy, and change in you know potential energy is zero. And no work interaction is taking place. And there is no heat interaction as well, and it is a flow open system, because some fuel and oxidizers is coming, getting burned and it is going out. But there might be a situation where the flow would not be taking place, are you getting my points?

So how to handle that you need to worry about, but we are now considering about flow passes in a burner. So if I apply this first law of thermodynamic, you know for determining the adiabatic temperature those things it will be sufficient or you need to know something more about is a sufficient. It will be sufficient provided if you know that product is CO 2 and water. But in real situation, it need not to for the simplicity sake, we are considering the product to be carbon dioxide and water. For the time being let us do that when we apply this first law of thermodynamics under the condition of you know assumption have stated just now for a control volume, you know or a open system that is H p is equal to H R.

And this is what will temperature will get is basically T adiabatic. This adiabatic will be because no heat is going out of the system, so all the heat will be there, so whatever temperature I will get, I will call it as a adiabatic temperature. So therefore the product will be depending on adiabatic will be function adiabatic temperature and pressure. Of course, pressure I am assuming it to be same as that of an inlet. Can I assume that pressure or it will be changing it will be changing or it will be remaining constant. What will happen, the pressure will be remaining almost constant, because it is a constant pressure passes we are assuming. And whatever heat of reaction, heat of reaction is basically n i h i, and n i is the number of moles participating reactant, in this case, it is a methane and oxidizer, where is a h i is the heat of formation of individual species.

And keep in mind that this heat of formation for individual species will be having what you call heat of the enthalpy of individual species will be having two components one is this is heat of formation at standard state, and this portion is known as sensible enthalpy we have studied in the last lecture. And this is integrated you know, it is a T naught to T particular temperature, because the T naught at which all the data will be given. All the heat of formation data will be given and C p keep in mind is a function of temperature. I can a take out, because temperature will be very high.

For example if you inlet temperature 298 Kelvin, what will be the adiabatic temperature, what will be the order. In case of a methane oxidizer, it will be very high, it will be around maybe 3000 Kelvin. If it is air, it will be lower, because nitrogen is there which is an inert gas. So therefore we cannot really assume that C p is a not a function of temperature or it is constant we cannot refer to do that this case what we are done earlier while handling the compressible flow. So similarly the total enthalpy of the product is summation of n i and h i; hi is the enthalpy of individual species and it is having two what you call term here one is heat of formation of this species is a product. And of course the sensible enthalpy keep in mind that this is being integrated from T naught that is the inlet temperature sorry that is the what you call the standard temperature T naught to be adiabatic. So what will do, we will just substitute this in this equation, you know if I look at this equation one, if I say this is the equation one if I was substitute H R and H P in this equation one, I will get an expression.

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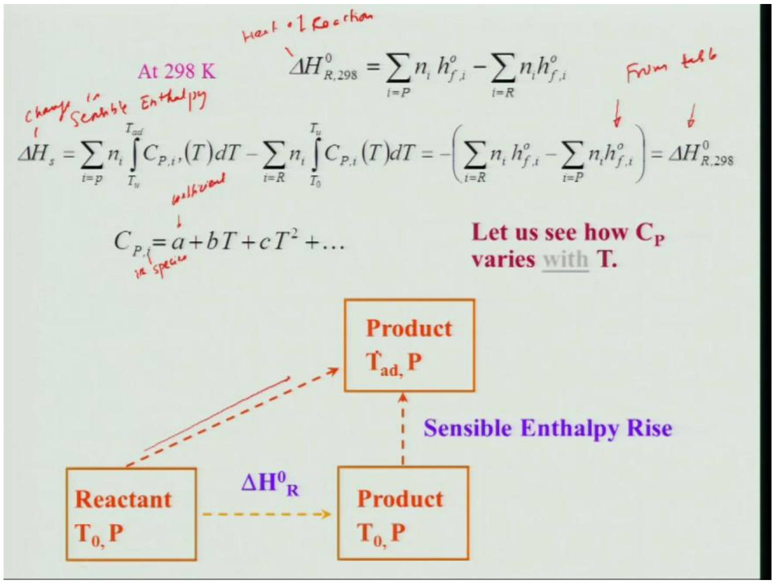

At 298 K

Heat of Reaction

$$\Delta H^0_{R,298} = \sum_{i=P} n_i h^o_{f,i} - \sum_{i=R} n_i h^o_{f,i}$$

From table

change in Sensible Enthalpy

$$\Delta H_s = \sum_{i=p} n_i \int_{T_u}^{T_{ad}} C_{P,i}(T)\,dT - \sum_{i=R} n_i \int_{T_0}^{T_u} C_{P,i}(T)\,dT = -\left(\sum_{i=R} n_i h^o_{f,i} - \sum_{i=P} n_i h^o_{f,i}\right) = \Delta H^0_{R,298}$$

without

$$C_{P,i} = a + bT + cT^2 + \dots$$

ith species

Let us see how C_P varies with T.

And then let us look at at 298 what we call this is basically heat of reaction, heat of reaction H r we know that by definition n i h f i with respect to standard condition. And similarly, for the reactant that is n i h f i with respect to standard condition this is our heat of reactant. If I substitute look at this equation one and substitute those values, we will get the sensible enthalpy, this is change in sensible enthalpy is equal to basically you know n i for the product and n i, I can take n Cp i T d T. And similarly, for the reactant, you know n i C p d T integrate over t naught T u and T u is to be adiabatic you know, because that is the inlet of the temperature what would be…

And which is equal to what, and this is the heat of reaction you know these portion that is the heat of reaction; that means this data I can get from what. Like if you look at this data heat of formation from table, I can get provided, I know what is n i that means each stoichiometric are the in a number of moles. If you look at I must know right for individual species then only I can get but we really know that in real situation we did not really know. And those things will be depended on temperature, for the simplicity sake I am again repeating that is, we will be use a assuming the product to be carbon dioxide, and water or something else, but it must be known for the time being we are assuming.

So when you do that then we can find out what will be T adiabatic provided, we know that how this C p is wherein, Cp is basically not only depended on the species. This is species, you know that is ieth species it can be methane, it can be oxygen, it can be carbon dioxide, it can be water anything. It will be depended on the temperature like these are coefficient, you know coefficient which are to be obtained from the table are particular species, and these are of course if polynomial being speed. And you will see that from table this will be valid for certain range this coefficient another set-of coefficient will be used for higher temperature, you know that you will see. Now let us just to say that you know it is a let us see that how this C p is varying with the temperature.

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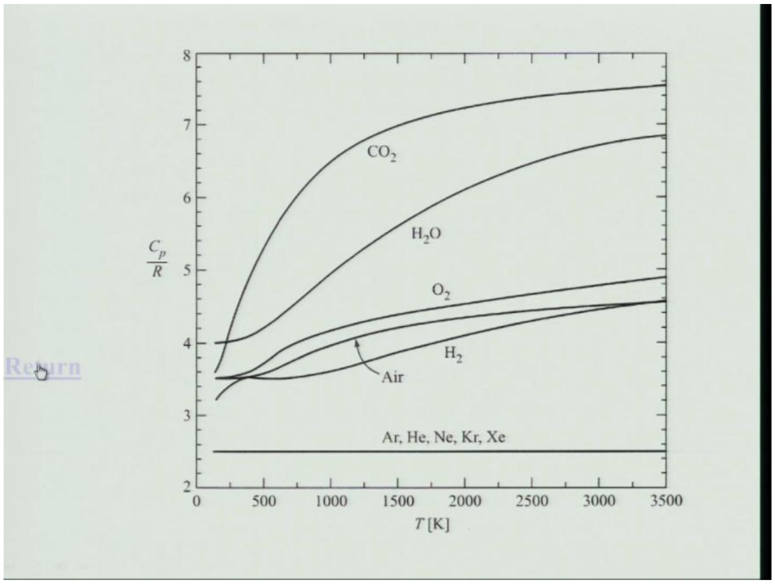

Let us look at a place if you look at Cp for the space is like hydrogen oxygen water carbon dioxide is varying with temperature of coarse four a mono atomic, you know molecule really it does not varies and we do not use this space is particularly for our combustion reaction. However we use to water oxygen hydrogen methane propane, all those things and several other species so we cannot afford to say that it is remaining constant whenever we are talking about you know combustion particularly where the temperature will be quite high of the change in temperature will be quite so you should keep in mind these things.

Now, what is the meaning of this you know what really we are doing if you look at that is the reactant is going to the product for the same temperature as a result some heat being relies right and these heat being utilized to an Hess's, this temperature the product to adiabatic. If you look at actual is it happening, just for the simplicity to make you understand what is happening have drawn that the actual passes is going in this way that means reactant is going to the product it having a temperature adiabatic higher temperature.

So you can think of the heat being release, and it is being you know the product the temperature is increase, it is sensible enthalpy raise, because is adiabatic passes. Even though it is non adiabatic steel, it will be increasing, but you will get a temperature which is low here than the adiabatic temperature. In case of some heat made be going in real system there is no adiabatic temperature aspect, it is just what you call theoretical one. Suppose I want to burn some fuel and oxidizer burner, can I get adiabatic temperature it is quite difficult because some heat has to be you know transfer to the atmosphere. Even though you can insulate but still some amount will be going out, you can add make insulation 100 right, as a result Q cannot be the heat transfer from the system cannot be release is zero, whatever you do so that is the reality.

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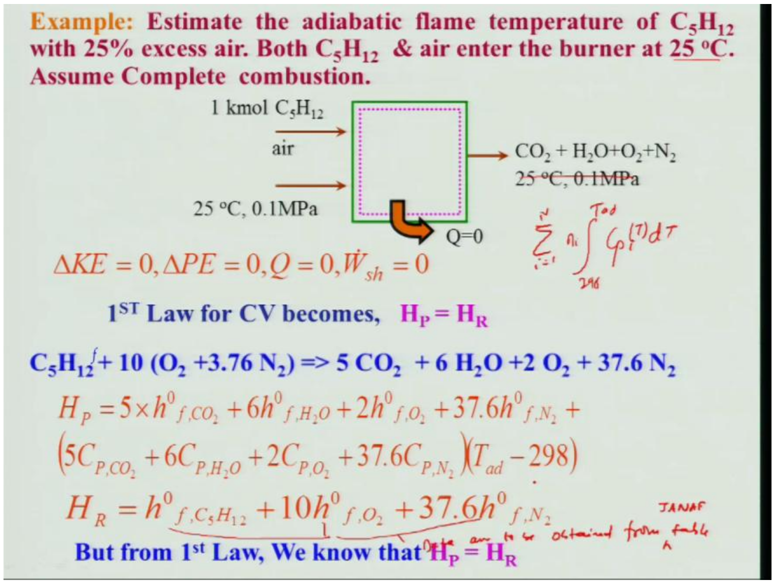

Example: **Estimate the adiabatic flame temperature of C_5H_{12} with 25% excess air. Both C_5H_{12} & air enter the burner at 25 °C. Assume Complete combustion.**

$$\sum_{i=1}^{N} n_i \int_{298}^{T_{ad}} C_{p,i}(T)\,dT$$

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

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

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

$$H_P = 5 \times h^0_{f,CO_2} + 6h^0_{f,H_2O} + 2h^0_{f,O_2} + 37.6h^0_{f,N_2} +$$
$$(5C_{P,CO_2} + 6C_{P,H_2O} + 2C_{P,O_2} + 37.6C_{P,N_2})(T_{ad} - 298)$$
$$H_R = \underbrace{h^0_{f,C_5H_{12}} + 10h^0_{f,O_2} + 37.6h^0_{f,N_2}}$$

these are to be obtained from JANAF table

But from 1^{st} Law, We know that $H_P = H_R$

And let us now take an example seeing that under this ideal condition ideal means in the sense, I do not know the composition right, but I am assuming certain composition and combustion of what combustion of product, and then estimating the temperature. And keep in mind the these composition will be depended on the final temperature that is adiabatic temperature that means they will be complementing each other. So which we do not know, so what will do we will you know estimate the adiabatic temperature of pentane 5 is C 5 H 12 with the excess of 25 percent air. Both is pentane and air enter at the 25 degree Celsius and assume the complete combustion that is again assumption we have doing. And we will do all these assumption change in kinetic, change in potential is zero and Q is zero there is no shaft work, so the first law becomes H P is equal to H R. And if you look at it this reaction is given and you can see that it is quite balanced some amount of oxygen is there in an excess oxygen, so what we will do basically products are given like carbon dioxide, water and the oxygen. And then this things so then we can really find out what is this H p.

If you look at it is having one components that is 5 h f of CO 2 that is your heat of formation term and 6 h f water that is the, you know for water and oxygen and also nitrogen beside this you know like it is having sensible enthalpy. And here what we are doing, you know we are saying that Cp is not really a you know, it is remaining constant in this example what if you look at this is Cp i d T, which is the function of temperature right ok and this is 298 two T adiabatic. Of course, there will be n i is equal to 12 n, this term we are now re-evaluating and keep in mind that what we are assuming here actually Cp is not changing over the range of temperature which is not true ok but for the to make the problem track tables we are assume.

And then what we will do, we will have to take a average temperature specific heat between the temperature; that is 298 to T adiabatic temperature which is basically will be little erroneous. But you know, we can solve the problem making a certain amount of error so that is why we have done, this is the very important assumption. Please keep in mind, then of course H r we know very easily that is h f this data are given, so this data is you know H and then this hf. And then this data can be obtained, you know data are to be obtained from table, which table this is j n f table, j n f table or as I told it is there on the backside of my book, so this data information heat of formation of individual basis. You can get very easily we will do that. So then from first law you know H p is equal to H r right and then substitute this H p and H r in that equation then we will get how to solve that.

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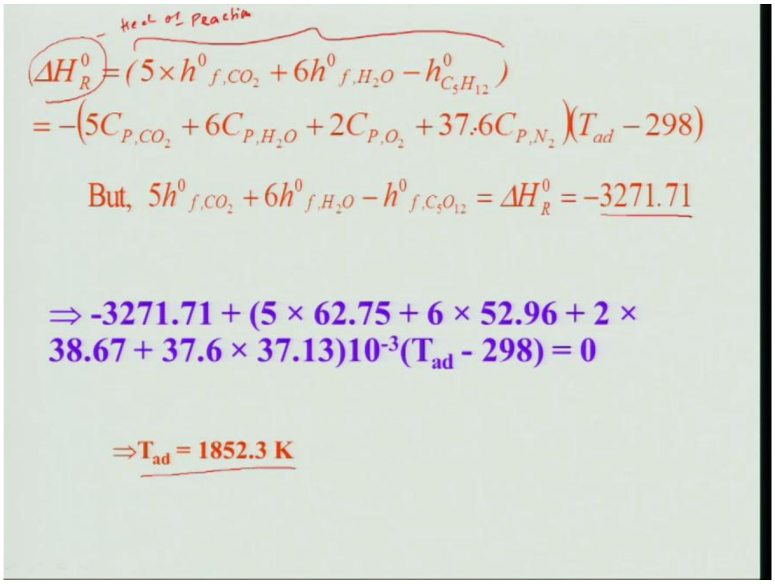

$$\Delta H_R^0 = \overbrace{(5 \times h^0_{f,CO_2} + 6h^0_{f,H_2O} - h^0_{C_5H_{12}})}^{\text{heat of Reaction}}$$

$$= -(5C_{P,CO_2} + 6C_{P,H_2O} + 2C_{P,O_2} + 37.6C_{P,N_2})(T_{ad} - 298)$$

But, $5h^0_{f,CO_2} + 6h^0_{f,H_2O} - h^0_{f,C_5O_{12}} = \Delta H_R^0 = -\underline{3271.71}$

$$\Rightarrow -3271.71 + (5 \times 62.75 + 6 \times 52.96 + 2 \times 38.67 + 37.6 \times 37.13)10^{-3}(T_{ad} - 298) = 0$$

$$\Rightarrow \underline{T_{ad} = 1852.3 \text{ K}}$$

So if you look at if I take this portion, and this what you call portion actually if you look at carbon dioxide and water this portion is nothing but your heat of reaction, this is heat of reaction. So which is no and then we will have to substitute this value of C p and this must be chosen properly values of C p, CO 2 water, and then oxygen nitrogen, otherwise you will land in getting a temperature which is quite different. So therefore, you know has to be it has to be choose in (( )), but from these heat of reaction, we can get this from the substituting this value and when we will choose this value. And we have taken for the C p, you know this is the Cp values for the carbon dioxide and this is for the water and this is for the O 2, you call O 2 and this values for the Cp values for nitrogen. And when we substitute this values and if you look at only unknown is T adiabatic, all are known, and this is a zero. So I will get a temperature which is 1852 .3 Kelvin, sometime you know this temperature would not mach with whenever will be using you know a software to estimate the adiabatic temperature.

And in the software, if you look at it will be taking care of the composition what will be the composition final composition. So and most we will be you know doing for this, this can be used by hand calculation, but it may be very away from the actual data unless otherwise you take the c p values properly that is very important, because we are making an assumption of taking a average temperature.

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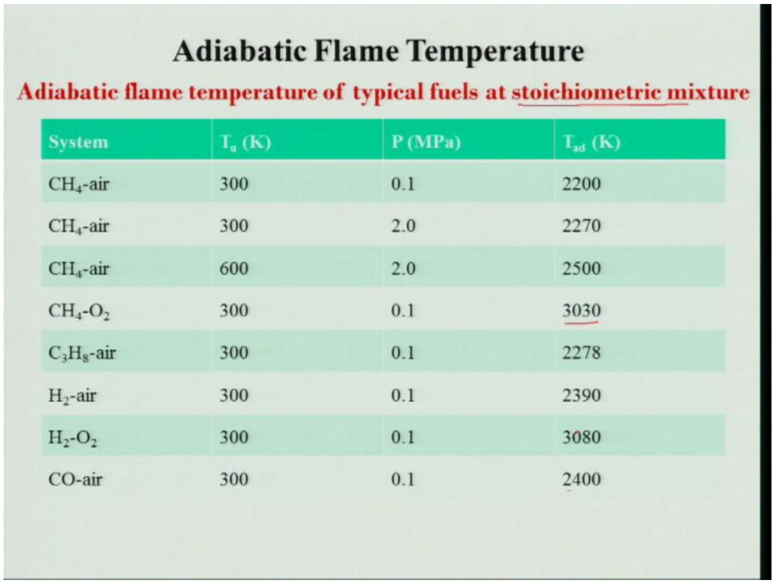

Adiabatic Flame Temperature

Adiabatic flame temperature of typical fuels at stoichiometric mixture

System	T_u (K)	P (MPa)	T_{ad} (K)
CH_4-air	300	0.1	2200
CH_4-air	300	2.0	2270
CH_4-air	600	2.0	2500
CH_4-O_2	300	0.1	3030
C_3H_8-air	300	0.1	2278
H_2-air	300	0.1	2390
H_2-O_2	300	0.1	3080
CO-air	300	0.1	2400

Let us look at how this adiabatic temperature which will be coming like if I look at the CH 4 air and that is stoichiometric mixture write only that is inlet temperature three hundred pressure is point one you can get 2200 Kelvin right. If I will increase this pressure to what happened the 2270 Kelvin. It is come from methane air, which is not really very much that means the temperature, you know pressure is not having much effect. But however will see it is having certain amount of, now if I will change this to the inlet temperature to 600 Kelvin, what you find. You will find almost 300 degree, you know kind of things with the respect to this, you know like around 230 Kelvin difference is there like generally people roughly say you are the inlet temperature to adiabatic temperature corresponding to the 298.300 Kelvin. We will get that I am in that is a roughly and if instead of air. If I use the oxygen what I get I get something 3030 Kelvin as compared to the 2200; that means I won not 830 different you get and if I look at propane you get 2278 Kelvin, if you look at most of the hydrocarbon of coarse this is stoichiometric mixture.

And we will be not varying, it will be over in around 2200 Kelvin. You should keep in mind roughly I mean 2200 to 2300 Kelvin in that range most of the hydrocarbon air. You know that a adiabatic whereas if I go for hydrogen you know it is having 2390 Kelvin and of course hydrogen oxygen will again go to the 3000 order and CO air is having 2400 this is quite interesting. How come it is having highly temperature as compared to the hydrocarbon but equally CO air is quite interesting. Still people has to be solved that and keep in mind that you may get a you know like this kind of why it is happening, you know interesting. So what you can learn from here it is that means adiabatic temperature dependent on pressure dependent on the inlet temperature, and also it is depended on the type of oxidized all the fuel were using except that hydrocarbon air which will be having almost you know to in the range of 2000 to 2300 Kelvin.

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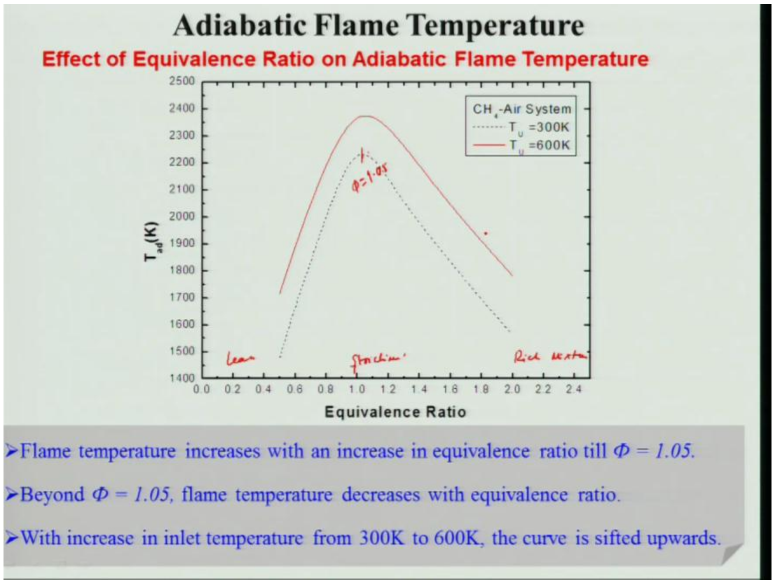

Adiabatic Flame Temperature

Effect of Equivalence Ratio on Adiabatic Flame Temperature

- Flame temperature increases with an increase in equivalence ratio till $\Phi = 1.05$.
- Beyond $\Phi = 1.05$, flame temperature decreases with equivalence ratio.
- With increase in inlet temperature from 300K to 600K, the curve is sifted upwards.

So let us look at how this is that means you know it will be depending on the inlet temperature, inlet pressure and also it will be depending on the fuel air ratio of equivalence ratio. Let us look at how it is really varying I have taken an example and methane air system with 300 Kelvin look at adiabatic temperature is plotted with the respect equivalence ratio right. If you look at what you are observing you are observing that temperature is increasing you know from the lean limit you know the lean mixture, this is the lean mixture right this is the rich mixture, and this is the of course the equivalence ratio 1 that is stoichiometric.

This is your stoichiometric this one right and this is increasing having a speed values over here again it is decreasing right that means it is increasing from the very lean mixture, and it is goes up and then again pick value. And then this weak value for hydrocarbon occurs around phi is equal to 1.05, and it decrease a keep in mind that slope is very steeper in the inside and on it is a little less. You know steeper as compared to the lean side on in the case of rich mixture right why it is so, it is a made it to be founder about it. And similarly, when you increase this inlet temperature 2600 Kelvin that is a red line which indicate the similar features and most of the hydrocarbon mixture will be having similar features, so all other hydrogen air and all these things.

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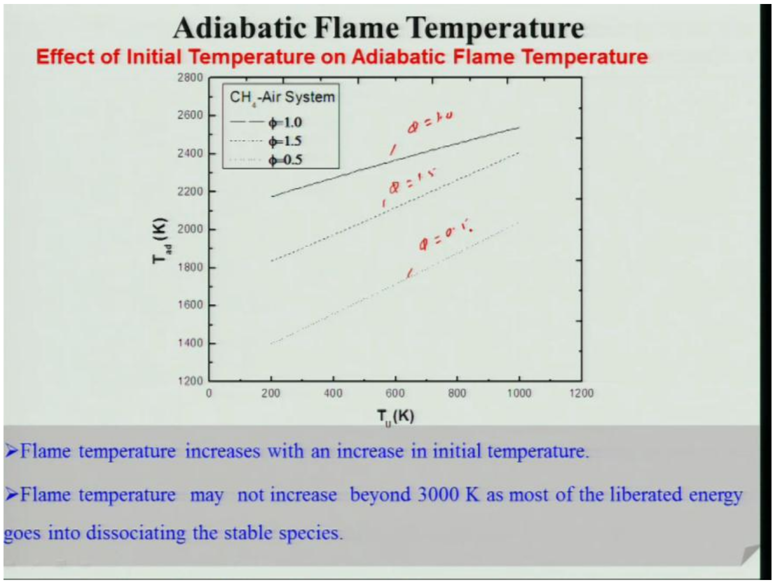

Adiabatic Flame Temperature

Effect of Initial Temperature on Adiabatic Flame Temperature

- Flame temperature increases with an increase in initial temperature.
- Flame temperature may not increase beyond 3000 K as most of the liberated energy goes into dissociating the stable species.

So let us now look at how it is you know varying with initial temperature, and if you look at I have taken a stroke you know three equivalence ratio methane air system one is of course the one this is the phi is equal to 1. And if you look at with inlet temperature, the adiabatic temperature just increasing and phi is equal to 1.5, this is phi is equal to 1.5 and this is phi is equal to 0.5. Of course, all are having similar features like it is and keeping mind as you go on, we cannot really go beyond the 3000 Kelvin, because the dissociation will be occurring. If the decision will occur then the temperature will be come back to the in around that number of 3000 R number.

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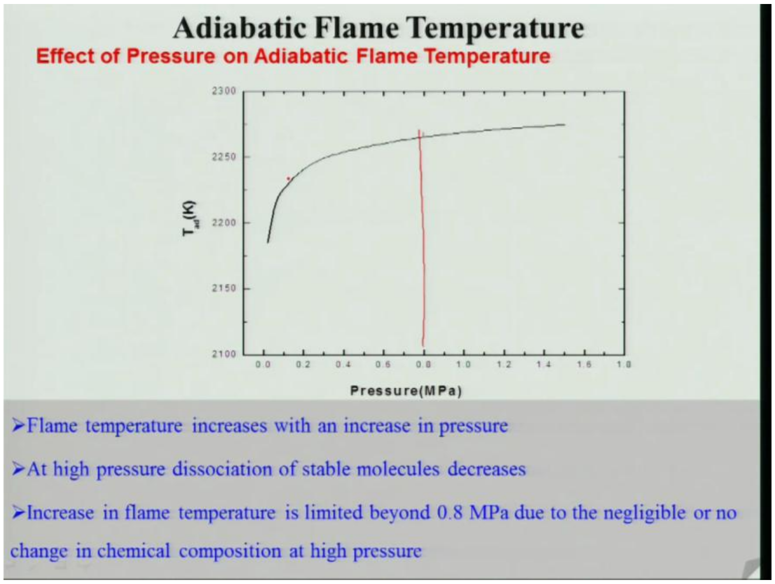

Adiabatic Flame Temperature

Effect of Pressure on Adiabatic Flame Temperature

- Flame temperature increases with an increase in pressure
- At high pressure dissociation of stable molecules decreases
- Increase in flame temperature is limited beyond 0.8 MPa due to the negligible or no change in chemical composition at high pressure

So let us see look at how this pressure you know that adiabatic temperature, if you look at it is at the lower pressure, it is increasing stiffly after that it is asymptotically increases and keep in mind that beyond 0.8 like kind of temperature. That is you know the temperature increase would not be very much due to the no change in chemical composition particularly high pressure. So, therefore I am like it is a high pressure or not really change in Mach but in the low pressure region you know there effect is very similar in the temperature.

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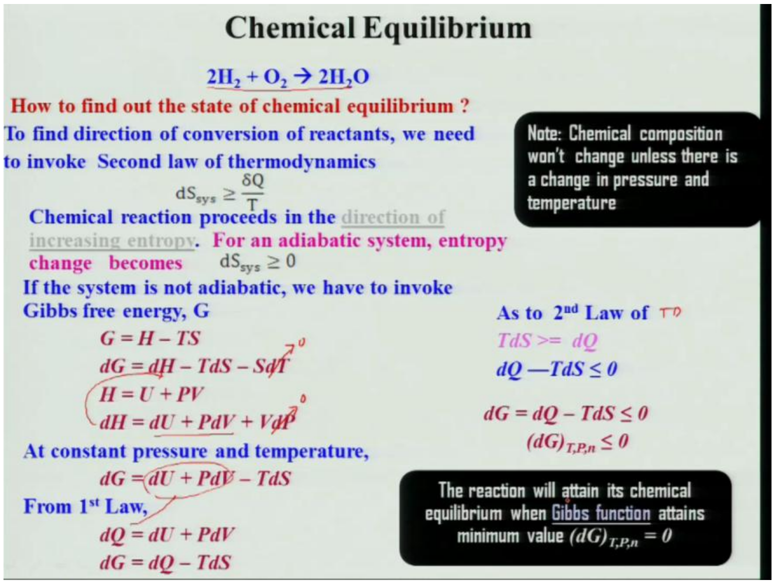

Chemical Equilibrium

$$2H_2 + O_2 \rightarrow 2H_2O$$

How to find out the state of chemical equilibrium ?

To find direction of conversion of reactants, we need to invoke Second law of thermodynamics

$$dS_{sys} \geq \frac{\delta Q}{T}$$

Chemical reaction proceeds in the direction of increasing entropy. For an adiabatic system, entropy change becomes $dS_{sys} \geq 0$

If the system is not adiabatic, we have to invoke Gibbs free energy, G

$$G = H - TS$$
$$dG = dH - TdS - S\cancelto{0}{dT}$$
$$H = U + PV$$
$$dH = dU + PdV + V\cancelto{0}{dP}$$

At constant pressure and temperature,

$$dG = dU + PdV - TdS$$

From 1st Law,

$$dQ = dU + PdV$$
$$dG = dQ - TdS$$

Note: Chemical composition won't change unless there is a change in pressure and temperature

As to 2nd Law of TD

$$TdS >= dQ$$
$$dQ - TdS \leq 0$$
$$dG = dQ - TdS \leq 0$$
$$(dG)_{T,P,n} \leq 0$$

The reaction will attain its chemical equilibrium when Gibbs function attains minimum value $(dG)_{T,P,n} = 0$

So, now what we have discussed till now about adiabatic temperature is ah that we assume the composition but whether we know this composition, and all right for example like if I take let's say hydrogen you know reacting with the oxygen. And we can always say it is going to the water for example if I take a container, and I put some hydrogen and oxygen right with a particular proportion you know what you call ratio right than what will happen can really reaction occurs. For example, if I take this room and fill with hydrogen and oxygen or air can really reaction takes place, it will go to the certainly no you need to ignite. Of course, if you even give they initially ignition energy with the all the hydrogen, all the oxygen will be going to the water you really I mean whether it is possible or not that will be depended on what in real situation it may not right. But of course if the you know pressure is constant so also the temperature is constant then composition chemical composition would not change.

However, how will determine, what will be the composition of you know the some reaction will be taking place, keep in mind that whatever the reaction, I have written here need not to be there in real situation. There might be several reaction states which will be there, which will be involved, and this is just you know global reaction or a representative reaction overall reactions, whatever it will be occurring. Now how to go about we are interested to know composition because our objective is to determine the adiabatic temperature unless I know the composition, I cannot estimate adiabatic temperature unless I know the adiabatic temperature I cannot estimate the composition, right product that means composition of the product.

So how to go about it, what we will have to we'll have two basically you know find out the state of equilibrium, how far it is reached equilibrium. Now question arises how to find out the state of equilibrium, because if it has gone you know some hydrogen is reacting and oxygen is going, and it is going in the forward direction to water. And water can also decompose into the oxygen or to the water hydrogen now what if I consider only this reaction. Of course in real situation, there might be several kind of reaction will be occurring, but I will just consider this reaction itself for the simplicity.

Now how will find out whether equilibrium reach, because it is equilibrium reach that means forward reaction will be same as the back out reaction rate. But how will go, how will say that it is whether it is possible or not. For that we need to invoke the second law thermodynamic right, because that will give us the direction of the reactant. You know whether it will be what is the percentage of reaction is converted, you know or it is the how much will be the product that for that we need to invoke second law of thermodynamics, which takes that change in entropic of this system must be greater than equal to the you know del Q by T right. This we have already studied and for adiabatic system what it would be right, it will be basically will be zero, changing entropy will be zero that means if it is greater than equal to zero, you know, then I can system can proceed otherwise no. For example like you went to see that whether chemical reaction proceeds in what you call in particular direction or not there will be increasing entropic or it will equal to the zero.

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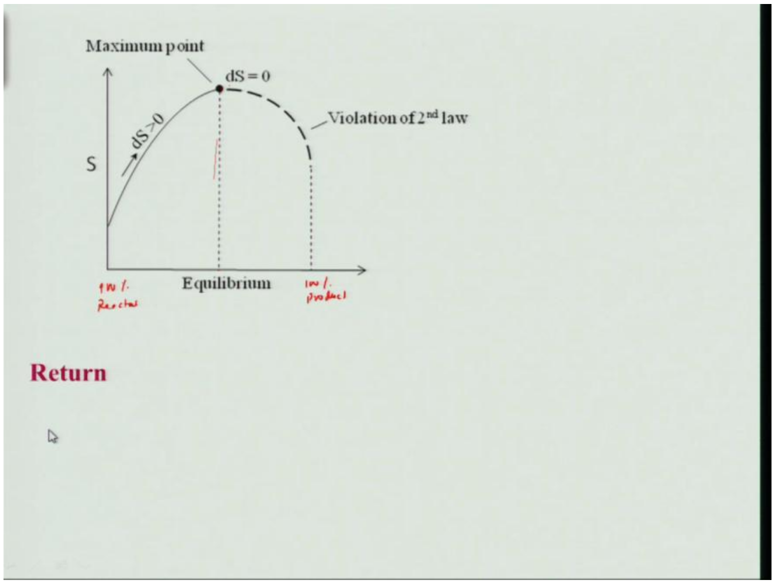

So, let us look at how this process takes place. For example if I say that this is hundred percent reactant, and this will be hundred percent product. For example I have taking the hydrogen reaction with oxygen reaction going to the product, so the reaction will proceed as long as the change in entropic is greater than zero. But it will go T reach at maximum points where there the change in entropic will be zero, and as this portion will be violating, you know second law thermodynamic. Therefore it cannot be really take place that means it will reach equilibrium composition when the change in entropic will be zero and that is valid only for what only for a adiabatic system.

But we know that in our this dumb, there will be you know several pressure, where need not to be a adiabatic. So then we need to think about you know a concept area which known as Gibbs free energy, we know by definition G is equal to h minus TS right and H is the enthalpy T is the temperature s is the entropic. So if I just differentiate what I will do, I will get this dG is equal to dH minus T dS right and minus S dT. And we know like you know the temperature, we need to remain constant I can make this as a zero like, you know whenever this equilibrium talking about H then by the deformation H is equal to U plus PV. And if i just differentiate this expiration H is equal to U plus PV, what I will get dH is equal to dU plus P dV and plus V dP and keep in mind that we are assuming that pressure you know during equilibrium is not changing, so this is basically zero. So if I just substitute this value, because that the constant pressure, and temperature this values over here what I will get that means dh is basically you plus P dV.

Then I will put over this then what I will get dG is equal to dU plus p dV minus T dS and if you look at what is this is term from the first law, we know that dQ is equal to dU plus P dV. So this term is nothing but dQ, so I can say that their dG is basically dQ minus T dS. So if I go to the according to the second law of thermodynamic, I can write down T dS is greater than equal to dQ or I can write down dQ minus T dS less than equal to zero. Because I am just saying this is greater than that that means dQ minus T dS you know will be less than equal to zero. And what is that this we have already seen dQ minus T dS that is nothing but dG is less than equal to zero. So what will have to do in case of non-adiabatic system, we can think of you know dG will be less than equal to zero that as a you know it is also a function of temperature and number of moles. We will be assuming the temperature and pressure is not real change in the moment, the reaction will attain its chemical equilibrium when Gibbs function you know attains the minimum value that is changing you know Gibbs function will be equal to zero.

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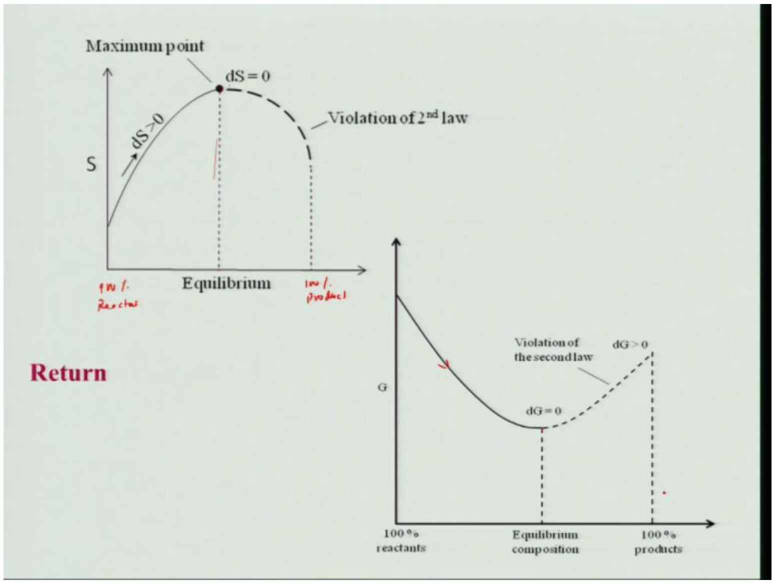

Return

Let us look at you know pictorially that is you know this is 100 percent reactant, and 100 percent product the process going on in the process. You know T literature this point which equilibrium composition; that means we need to estimate you know equilibrium composition dG, and here this is not possible in this portion that means because it will be violating the second law of thermodynamic. And therefore, we cannot really get hundred percent product in real situation, and we will see that these concept will be using the next class and see that how can get that composition. Then of course, after that I will be moving into the chemical kinetics, and we will also learn how this composition can be cloud to estimate the adiabatic temperature; that means in a very heated temperature that will see in the next class.