

Turbulent Combustion: Theory and Modeling
Prof. Ashok De
Department of Aerospace Engineering
Indian Institute of Technology-Kanpur

Lecture-5
Thermo-Chemistry (Contd..)

Welcome back. Let us continue our discussion on turbulent combustion and we are discussing now combustion and thermochemistry and where we stopped in the last class when we are having a reacting system with multiple species. So we looked at different properties and how to calculate them and we stopped where we looked at the calculation of the total pressure.

(Refer Slide Time: 00:39)

1: Combustion & Thermochemistry

total pressure $\rightarrow P = \sum_i P_i$, $P_i =$ partial pressure of i^{th} species
 $P_i = X_i P$ - - - (1.14)

For ideal gas mixtures:
 $h_{\text{mix}} = \sum_i Y_i h_i$ - - - (1.15a)
 $\bar{h}_{\text{mix}} = \sum_i X_i \bar{h}_i$ - - - (1.15b)

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 72

So, this is where we had it. The total pressure would be the summation of the all the partial pressure where P_i is the partial pressure so that is how you get the total pressure of the system. So this will give you the total pressure of the system now and partial pressure of i^{th} species. So, individual species partial pressure is summed up to get the total pressure of the system. Now how partial pressure we can find out or rather. We can find out renamed from partial pressure. If we know the total pressure of the system, then we can actually find out the partial pressure of that individual species.

So to find out that where you know the total pressure you can find out with the mole fraction into

total pressure, so that will get you the partial pressure of the individual species. Now, we are dealing with the ideal gas mixture so for ideal gas mixture you can get:

$$h_{mix} = \sum_i Y_i h_i$$

So, let us continue what the similar notation of the equation system. So this should be 1.15a and the mean would be:

$$\bar{h}_{mix} = \sum_i Y_i \bar{h}_i$$

So this is 1.15b so that is how you get individual these things.

(Refer Slide Time: 02:51)

1: Combustion & Thermochemistry

$$S_{mix}(T, P) = \sum_i Y_i S_i(T, P) \dots (1.16 a)$$

$$\bar{S}_{mix}(T, P) = \sum_i X_i \bar{S}_i(T, P) \dots (1.16 b)$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 73

Now similarly, you can find out the entropy. So for example, entropy is a function of temperature and pressure so that will get you if you get summation over all the species i then Mass fraction of individual species S_i , temperature pressure so that you say 1.16a then similarly you can find the average entropy who should be again similarly like overall X_i average entropy and that would be your 1.16b. Now, pure species entropy depends on the species partial pressure, which you can see from this above equation. So you can use this and get the different equations.

(Refer Slide Time: 03:59)

1: Combustion & Thermochemistry

$$P_{ref} = P^\circ = 1 \text{ atm} \quad (\text{standard state})$$
$$S_i(T, P_i) = S_i(T, P_{ref}) - R \cdot \ln \frac{P_i}{P_{ref}} \quad (1.17a)$$
$$\bar{S}_i(T, P_i) = \bar{S}_i(T, P_{ref}) - R \cdot \ln \frac{P_i}{P_{ref}} \quad (1.17b)$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 74

Now, if you take a reference state, let us say reference state is P^0 which is 1 atm. So, if you take a standard state that also one can say this is an standard state so and that is what you take as a reference state and you calculate S_i for a particular partial pressure P_i which will be:

$$S_i(T, P_i) = S_i(T, P_{ref}) - R \cdot \ln \frac{P_i}{P_{ref}}$$

That is why we are actually to some extent doing the revision of our basic thermodynamics along with the combustion. So this would be 1.17a. Let us say a then the average one you can find out for P_i , would be:

$$\bar{S}_i(T, P_i) = \bar{S}_i(T, P_{ref}) - R \cdot \ln \frac{P_i}{P_{ref}}$$

So this would be one can look at that the individual calculation of these species and their entropy is and all these other properties.

(Refer Slide Time: 05:32)

1: Combustion & Thermochemistry

Enthalpy of vaporization:
P = const. process , h_{fg} = heat required

$$h_{fg} \equiv h_{\text{vapor}}(T, P) - h_{\text{liq.}}(T, P) \quad \dots (1.18)$$

Clausius - Clapeyron eq:

$$\frac{dP_{\text{sat}}}{P_{\text{sat}}} = \frac{h_{fg}}{R} \frac{dT}{T_{\text{sat}}^2} \quad \dots (1.19)$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 75

Now there would be another thing is that latent heat or enthalpy of vaporization. So, this is important when the liquid actually vaporizes. So for example, let us say P is constant pressure process then h_{fg} would be heat required so that is heat required to completely vaporize a unit mass of liquid at a given temperature. So, this is a constant pressure process and h_{fg} is the amount of heat, which is required to completely vaporize a unit mass of liquid at a given temperature.

So what we can get:

$$h_{fg} = h_{\text{vapor}}(T, P) - h_{\text{liq}}(T, P)$$

Now on one of the famous relation is Clausius-Clapeyron equation, which gives you an equation for saturated pressure with the enthalpy $\left(\frac{dT}{T_{\text{sat}}^2}\right)$. So, this is what you get from the Clausius-Clapeyron relation and that is what you can get and find out the amount of heat required or the enthalpy of vaporization.

(Refer Slide Time: 07:35)

1: Combustion & Thermochemistry

First Law of Thermodynamics:

First Law - Fixed Mass:

- Conservation of energy is the fundamental principle in the first law of thermodynamics. For a fixed mass system, energy conservation is expressed for a finite change between two states, 1 and 2, as:

$$\underbrace{{}_1Q_2}_{\text{Heat added to the system}} - \underbrace{{}_1W_2}_{\text{Work done by the system}} = \underbrace{\Delta E_{1-2}}_{\text{Change in total energy of system}} \quad (1.20)$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 76

So now we move to the first law of the system. So again, this is again the revision of thermodynamics. So first law of thermodynamics, which talks about essentially the fundamental principle of conservation of energy, so it talks about the energy for an isolated fixed Mass system. So, if you look at the finite change between State 1 and 2, so this is the equation which comes out of the first law or energy conservation. So that is the heat added to the system. So we follow some convention.

If heat is added then it is positive. So if this is the system it heat added it should be positive if it is the work done that would be positive. So this is work done by the system is the change in the energy of the system. So that is the ΔE .

(Refer Slide Time: 08:34)

1: Combustion & Thermochemistry

First Law - Fixed Mass (Cont'd):

- Both ${}_1Q_2$ and ${}_1W_2$ are path functions and occur only at the system boundaries. $\Delta E_{1-2} \equiv E_2 - E_1$ is the change in the total energy of the system, i.e.

$$E = m \left[\underbrace{u}_{\text{system internal energy}} + \underbrace{(1/2)v^2}_{\text{system kinetic energy}} + \underbrace{gz}_{\text{system potential energy}} \right] \quad (2.21)$$

The system energy is a state variable and does not depend on the path taken.

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 77

So, one important thing to note here both this heat and work they are path functions. So, there are two different kind of function that you come across there are few which point function but this is heat and work. These are essentially the path functions and this will only occur at the system boundary. So that is very, very important that where does it occur and that is the difference between total energy of the system. So, one can write the energy is a collection of all other energy source system. So you can have the internal energy you can have the kinetic energy and the potential energy. So, this will get to the total energy of that particular system and you have that system.

(Refer Slide Time: 09:30)

1: Combustion & Thermochemistry

First Law - Fixed Mass (Cont'd):

- We can write Eq 1.20 as a unit mass basis, or expressed to represent an instant in time:

$$\rightarrow \boxed{{}_1q_2 - {}_1w_2 = \Delta e_{1-2} = e_2 - e_1} \quad (1.22)$$

Rate form

$$\left\{ \begin{array}{l} \underbrace{\dot{Q}}_{\text{instantaneous rate of heat transferred}} - \underbrace{\dot{W}}_{\text{instantaneous rate of work done}} = \underbrace{dE/dt}_{\text{instantaneous change of system energy}} \end{array} \right. \quad (1.23)$$

per unit mass

$$\left\{ \begin{array}{l} \dot{q} - \dot{w} = de/dt \end{array} \right. \quad (1.24)$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 78

And you have the system now one can write the equation the first energy balance equation for unit Mass basis. So, one can get there are two ways one can write either unit mass basis then the difference between two state is the q_{12} , work done by the system w_{12} and that is the change of the energy. See this is still your first law energy conservation and same thing if one write in this is in rate form that means with respect to time if someone writes that energy balance, so this is the amount of heat transfer takes place across the system boundary.

Then the work done across the system boundary or rather at a rate of that system boundary and then this would be the change of the system energy. So, that would also with respect to time you get it and if you write per unit Mass this is in rate form per unit mass the energy conservation principal.

(Refer Slide Time: 10:59)

1: Combustion & Thermochemistry

First Law - Control Volume:

- Steady-state, steady-flow form of the first law:

$$\underbrace{\dot{Q}_{cv}}_{\text{Rate of heat transferred from surroundings}} - \underbrace{\dot{W}_{cv}}_{\text{Rate of work done by control volume excluding flow work}} = \underbrace{\dot{m}e_o}_{\text{Rate of energy flow out of CV}}$$

$$- \underbrace{\dot{m}e_i}_{\text{Rate of energy flow into CV}} + \underbrace{\dot{m}(P_o v_o - P_i v_i)}_{\text{Net rate of work associated with pressure forces}} \quad (1.25)$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR
Ashoke De 79

Now if we extend this one this first law analysis for the control volume system. So, these are again refreshing the memory of our thermodynamics because these are essential component of the detailed analysis what we are going to do later stage of this course. So, control volume analysis, you say steady state, steady flow from the first law. Then you have a control volume which is defined and across that control volume, this is your control volume.

Then you find out the rate transform, this is the heat rate, the work then rate of energy flow into

the control volume. So there will be a flux, change in flux. So something comes, in something goes out. So let us say e_i comes in e_o goes out with a mass. So, when you come to the control volume, there is a mass crossing the boundary then \dot{m}_{net} rate of the work a suit with the pressure forces so that you take into account then you get this equation for your steady state.

(Refer Slide Time: 12:21)

1: Combustion & Thermochemistry

First Law - Control Volume (Cont'd):

- Main assumptions in the previous equation:
 - The control volume is fixed relative to the coordinate system.
 - The properties of the fluid at each point within CV, or on the control surface, do not vary with time.
 - Fluid properties are uniform over inlet and outlet areas.
 - There is only one inlet and one outlet stream.

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 80

So, say there are certain assumptions which are associated with these particular equations. One of the important assumptions is that the control volume is fixed relative to the coordinate system. That means that is not moving. So once you have a fixed control volume that means it is fixed in space. Then the properties within the control volume they are not varying with time and that is why we assume it is a steady state.

So that means within that they are not changing with time. Also fluid properties they are uniform over Inlet and Outlet areas and all you have only one Inlet and one Outlet stream. So these are some of the assumption that we have to come to this particular equation for a control volume.

(Refer Slide Time: 13:17)

1: Combustion & Thermochemistry

First Law - Control Volume (Cont'd):

- Specific energy e of the inlet and outlet stream consist of:

$$\underbrace{e}_{\substack{\text{Total} \\ \text{energy per} \\ \text{unit mass}}} = \underbrace{u}_{\substack{\text{Internal} \\ \text{energy per} \\ \text{unit mass}}} + \underbrace{(1/2)v^2}_{\substack{\text{Kinetic} \\ \text{energy per} \\ \text{unit mass}}} + \underbrace{gz}_{\substack{\text{Potential} \\ \text{energy per} \\ \text{unit mass}}} \quad (1.26)$$

v = velocity where the stream crosses the CV
 z = elevation where stream crosses the CV
 g = gravitational acceleration

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 81

Now we can use the specific energy for the inlet and outlet stream. And what does that have? So as we have seen that specific energy, the total specific energy per unit mass will have a one component from the internal energy the same component. If one of these particular part of the component is not present in a system so that will not contribute otherwise the total energy or total specific energy should be coming from internal energy, kinetic energy and the potential energy.

And where your v is the velocity stream crosses the central control volume. Then this z is the elevation question cross the central volume and g is the gravitational acceleration. So these are standard terminologies which are used.

(Refer Slide Time: 14:15)

1: Combustion & Thermochemistry

Enthalpy: $h \equiv u + Pv = u + \frac{P}{\rho}$ -- (1.27)

(1.25 - 1.27) \Rightarrow

$$\dot{Q}_{cv} - \dot{W}_{cv} = \dot{m} \left[(h_0 - h_i) + \frac{1}{2} (V_0^2 - V_i^2) + g(z_0 - z_i) \right]$$

-- (1.28)

$$q_{cv} - w_{cv} = (h_0 - h_i) + \frac{1}{2} (V_0^2 - V_i^2) + g(z_0 - z_i)$$

-- (1.29)

INDIAN INSTITUTE OF TECHNOLOGY KANPUR
Ashoke De 82

Now similarly you can define other properties like enthalpy. So, specific enthalpy would be:

$$h = u + Pv$$

So, which you can write:

$$h = u + P/\rho$$

So then the prior is using couple previous equations, like 1.25 to 1.27. If you combine all of them, which will essentially get you:

$$\dot{Q}_{cv} - \dot{W}_{cv} = \dot{m} \left[(h_0 - h_i) + \frac{1}{2} (V_0^2 - V_i^2) + g(z_0 - z_i) \right]$$

So, difference of two different state.

So, again, this is the including all the masses if you look at per unit mass, so this will be represented as:

$$q_{cv} - w_{cv} = \left[(h_0 - h_i) + \frac{1}{2} (V_0^2 - V_i^2) + g(z_0 - z_i) \right]$$

So which will be your equation number 1.29, so you can write using the; you can bring in this enthalpy into the picture which will make your life quite easier.

(Refer Slide Time: 16:20)

1: Combustion & Thermochemistry

Reactant and Product Mixtures:

Stoichiometry:

- The stoichiometric quantity of oxidizer is just that amount needed to completely burn a quantity of fuel. For a hydrocarbon fuel, C_xH_y , stoichiometric relation is

$$\left. \begin{array}{l} C_xH_y + a(O_2 + 3.76N_2) \rightarrow \\ xCO_2 + (y/2)H_2O + 3.76aN_2 \end{array} \right\} \text{ (1.30)}$$

where $a = x + y/4$ (1.31)

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 83

Now if you move ahead and look at these things; the reactant and the product mixture, so one thing that we want to define is the stoichiometry. Now the stoichiometry quantity of oxidizer when you say that a particular reaction is a stoichiometric reaction so you can see this is one hydrocarbon, which is burned with here. Then you get CO_2 , H_2O , N_x is nitrogen, if nitrogen being an inert gas.

So, you can find out the balancing and get those numbers a, x, y everything and when you share that the equation is stoichiometry that means it is an sufficient or it is in balance between oxidizer and fuel which is required to for a particularly this compound to bond with the air that a amount of air is required which is enough to burn the completely fuel.

(Refer Slide Time: 17:22)

1: Combustion & Thermochemistry

$$\left(\frac{A}{F}\right)_{stoic} = \left(\frac{m_{air}}{m_{fuel}}\right) = \frac{4.76a}{1} \frac{MW_{air}}{MW_{fuel}} \dots (1.32)$$
$$\phi = \frac{\left(\frac{A}{F}\right)_{stoic}}{\left(\frac{A}{F}\right)_{act}} = \frac{\left(\frac{F}{A}\right)_{act}}{\left(\frac{F}{A}\right)_{stoic}} \dots (1.33)$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 84

So, air fuel ratio, you can find out the stoichiometric air fuel ratio. Let us say for which it would be:

$$\left(\frac{A}{F}\right)_{stoic} = \frac{m_{air}}{m_{fuel}} = \frac{4.76a}{1} \frac{MW_{air}}{MW_{fuel}}$$

The equivalence ratio, which is defined as:

$$\phi = \frac{\left(\frac{A}{F}\right)_{stoic}}{\left(\frac{A}{F}\right)_{act}} = \frac{\left(\frac{F}{A}\right)_{act}}{\left(\frac{F}{A}\right)_{stoic}}$$

Either way they would lead to the same set of expression.

(Refer Slide Time: 18:19)

1: Combustion & Thermochemistry

$\phi > 1$: Fuel-rich mixtures
 $\phi < 1$: Fuel-lean mixtures
 $\phi = 1$: Stoichiometric mixture

% stoichiometric air = $100\% / \phi$. . . (1.33 b)

% excess air = $\left[\frac{(1-\phi)}{\phi} \right] \cdot 100\%$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 85

And then you say ϕ greater than 1 that would be one condition ϕ less than 1 would be another condition ϕ equals to 1 would be one condition. So, obviously when ϕ equals to 1 means that is my actual fuel-air ratio and stoichiometry fuel-air ratio they are same so that means it is in balanced amount of fuel and oxidizer are there to have a combustion to take place. So, this is your essentially stoichiometric mixture.

Then when ϕ less than 1 you will have fuel-lean mixture and automatically this should be fuel-rich mixture and one can look at from the equation that we have derived here that what would be corresponding. Now another thing is that percentage of stoichiometric air percentage is here. So that is another definition:

$$\% \text{ stoichiometric air} = 100\% / \phi$$

So this is an percentage of excess air would be:

$$\% \text{ excess air} = \left[\frac{(1 - \phi)}{\phi} \right] \cdot 100\%$$

So this is what you can get.

(Refer Slide Time: 20:09)

1: Combustion & Thermochemistry

Absolute (or Standardized) Enthalpy and Enthalpy of Formation:

- For any species, we can define an *absolute enthalpy* that is the sum of an *enthalpy of formation* and *sensible enthalpy change*:

$$\underbrace{\bar{h}_i(T)}_{\text{absolute enthalpy at temperature } T} = \underbrace{\bar{h}_{f,i}^{\circ}(T_{\text{ref}})}_{\text{enthalpy of formation at standard ref state } (T_{\text{ref}}, P^{\circ})} + \underbrace{\Delta\bar{h}_{s,i}(T_{\text{ref}})}_{\text{sensible enthalpy change in going from } T_{\text{ref}} \text{ to } T} \quad (1.34)$$

where $\Delta\bar{h}_{s,i} \equiv \bar{h}_i(T) - \bar{h}_{f,i}^{\circ}(T_{\text{ref}})$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 86

Now second important thing is that absolute enthalpy and so that is one important terminologies absolute enthalpy, another is the enthalpy of formation. Now, absolutely enthalpy is some of an enthalpy of formation and sensible enthalpy. So this is how we get that means this is my total absolute enthalpy at a particular given temperature T. So that will have two component one component would contribute from the enthalpy of formation of a particular species.

That is why i comes here into this particular system or equation for a particular T reference and then the sensible enthalpy component, which is nothing but the energy required to have a change from T_{ref} to T. So, to go from one state to and this is the energy change or enthalpy change and that would be at a particular T. What is of concern:

$$\Delta\bar{h}_{s,i} = \bar{h}_i(T) - \bar{h}_{f,i}^{\circ}(T_{\text{ref}})$$

So this is how one would get these things.

(Refer Slide Time: 21:36)

1: Combustion & Thermochemistry

Absolute (or Standardized) Enthalpy (Cont'd):

- Define a standard reference state.
 $T_{\text{ref}} = 298.15\text{K}$ (25 °C)
 $P_{\text{ref}} = P^{\circ} = 1\text{atm}$ (101.325 kPa)
- Enthalpies of formation are zero for the elements in their naturally occurring state at the reference temperature and pressure.
- For example, at 25 °C and 1 atm, oxygen exists as diatomic molecules; then

$$(\bar{h}_{f,\text{O}_2}^{\circ})_{298} = 0$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 87

Now, how we define? We can define the standard state typically 25 degree centigrade and reference pressure one atm. So, enthalpy of formation are essentially zero for the elements in the naturally occurring state at the reference temperature and pressure. For example at one atmospheric pressure and 25 degree Centigrade oxygen exist as and 1 Atomic molecule. So the enthalpy of formation is 0 so there are plenty of similar things. I mean similar species like nitrogen, hydrogen other available. And one can refer to any of these textbook to look at the enthalpy of formation.

(Refer Slide Time: 22:20)

1: Combustion & Thermochemistry

Absolute (or Standardized) Enthalpy (Cont'd):

- To form oxygen atoms at the standard state requires breaking of a chemical bond.
- The bond dissociation energy of O_2 at standard state is 498,390 kJ/kmol.
- Breaking of the bond creates two O atoms; therefore the *enthalpy of formation* of atomic oxygen is

$0_2 \rightarrow 2\text{O}$

$$(\bar{h}_{f,\text{O}}^{\circ})_{298} = 249,195 \text{ kJ/kmol}$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 88

Now, what do you talk about absolute enthalpy? So the absolute enthalpy is the energy to form oxygen atom at the standard state requires breaking of chemical bond. And the bond dissociation energy of oxygen at standard state is this, this is a standard information one can; so the breaking of bond breaking a bond creates two oxygen atom. Therefore the enthalpy of formation of the oxygen is this, so what you get the enthalpy of formation, is that to break this O to 2O atoms.

So, this is the energy which is provided to break this bonding and you get the atoms here and that is what the enthalpy of formation is.

(Refer Slide Time: 23:15)


1: Combustion & Thermochemistry

Enthalpy of Formation (Cont'd):

- Thus, enthalpies of formation is the net change in enthalpy associated with breaking the chemical bonds of the standard state elements and forming new bonds to create the compound of interest.
- Examples:

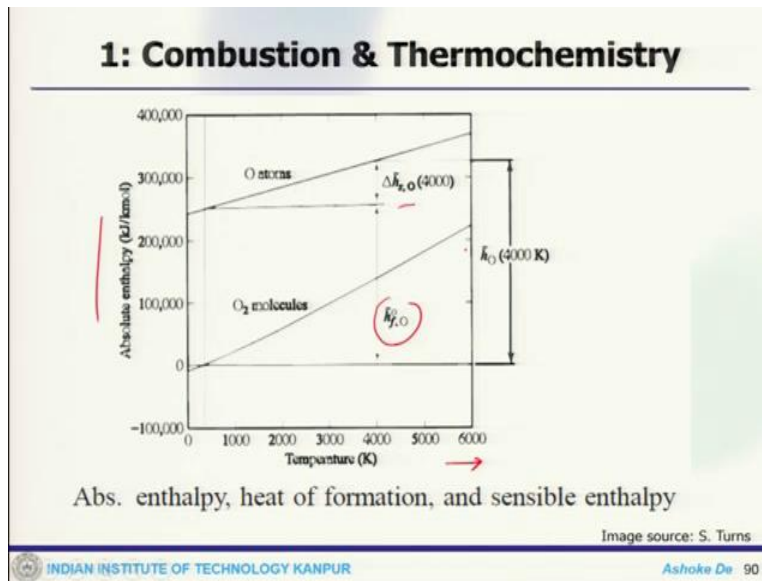
$$\left. \begin{aligned} (\bar{h}_{f,N_2}^{\circ})_{298} &= 0 \\ (\bar{h}_{f,H_2}^{\circ})_{298} &= 0 \end{aligned} \right\}$$

$$\left. \begin{aligned} (\bar{h}_{f,N}^{\circ})_{298} &= 472,629 \text{ kJ/kmol} \\ (\bar{h}_{f,H}^{\circ})_{298} &= 217,977 \text{ kJ/kmol} \end{aligned} \right\}$$

 INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 89

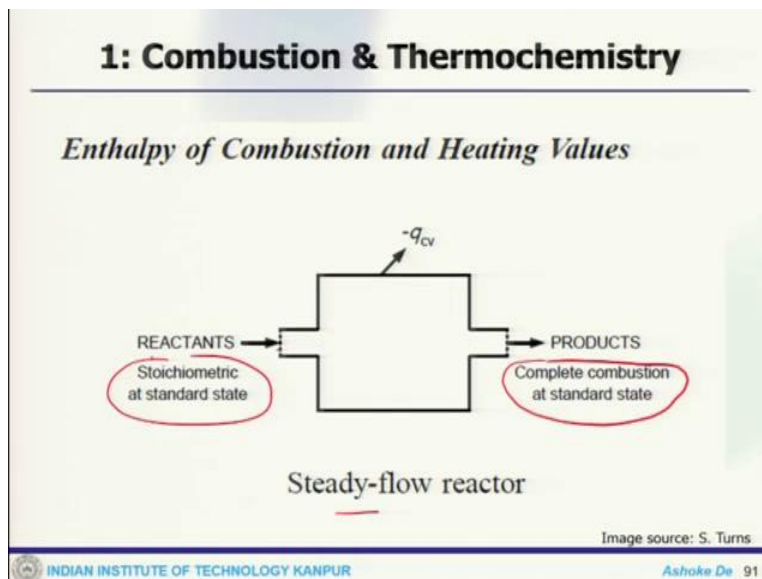
So, you can think about the enthalpy of formation is the Net change in enthalpy. So, one can write in really in takes the net change in enthalpy which is associated with breaking the chemical bonds of the standard state elements and forming new bonds. To create the compound of interest for example at standard state nitrogen hydrogen, they are 0 but if you look at N or hydrogen atom there are some enthalpy of formation. So this is a piece of information one can get in a book.

(Refer Slide Time: 23:54)



So this is one of the gap which gives you an idea that this side your absolute enthalpy. This is your temperature variation along these things. So this is oxygen molecule. This is oxygen atom and you can get the different situation this is your enthalpy of formation. And this is the change of state which is shown by that gap.

(Refer Slide Time: 24:27)



Now we move forward to look at the heating values or something, which is very common in combustion process is the enthalpy of combustion. So you have a system like this, is not it you think about a steady flow reactor? So there are reactants which are coming in through this inlet

and the product which are going out of this outlet where you assume there is a complete combustion at standard state that means the products which are going out they are the outcome of the complete combustion and reactants which are coming at the stoichiometric standard state.

(Refer Slide Time: 25:10)

1: Combustion & Thermochemistry

Enthalpy of Combustion and Heating Values (Cont'd)

- Reactants: stoichiometric mixture at standard state conditions.
- Products: complete combustion, and products are at standard state conditions.
- For products to exit at the same T as the reactants, heat must be removed.
- The amount of heat removed can be related to the reactant and product absolute enthalpies by applying the steady-flow form of the first law:

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 92

Now as I said stoichiometric mixture, the reactants at standard state products are the product of complete combustion. That means there is no excess fuel neither excess oxygen nor air which is oxidizer present there. But that also comes out at the standard state. Now prepare to exit at the same T and the reactants heat must be removed. So this is what exactly shown there because the reactants are coming at standard state and products are also coming out of standard state.

So that means the temperature but there is a reaction or combustion takes place here and when there is a combustion takes place there would be a amount of heat which is produced now that should be removed from the system to maintain that, so that would be related and product of the absolute enthalpy.

(Refer Slide Time: 26:02)

1: Combustion & Thermochemistry

Enthalpy of Combustion and Heating Values (Cont'd):

From eqn 1.29:

$$q_{cv} = h_o - h_i = h_{prod} - h_{reac} \quad (1.35)$$

- The enthalpy of reaction, or the enthalpy of combustion, Δh_R , is (per mass of mixture)

$$\Delta h_R \equiv q_{cv} = h_{prod} - h_{reac} \quad (1.36a)$$

or, in terms of extensive properties

$$\Delta H_R = H_{prod} - H_{reac} \quad (1.36b)$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 93

And you can use the first law here to find out that so the Amount of heat, which is there that is a difference between enthalpy of the outlet and the inlet. So that is the product enthalpy and the reactant enthalpy. Now the enthalpy of reaction or enthalpy of combustion so that is per mass of mixture one can say:

$$\Delta h_R = q_{ev} = h_{prod} - h_{reac}$$

Now in terms of extensive property, so if it is not per unit mass, so that is:

$$\Delta H_R = H_{prod} - H_{reac}$$

(Refer Slide Time: 27:08)

1: Combustion & Thermochemistry

Enthalpy of Combustion and Heating Values (Cont'd):

- Example:
 - At standard state, the reactants enthalpy of a stoichiometric mixture of CH₄ and air, where 1 kmol of fuel reacts, is -74,831 kJ.
 - At the same conditions, the combustion products have an absolute enthalpy of -877,236 kJ.

Enthalpy of reaction / combustion }
$$\Delta H_R = -877,236 - (-74,831)$$
$$= -802,405 \text{ kJ}$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR Ashoke De 94

So, we can take an example and see what happens. So let us say at standard state the reactants of stoichiometric mixture of methane and here where one kilo mole of fuel reacts is this. Now at the same condition, the combustion product have an absolute enthalpy of this. So, you get the ΔH_R or enthalpy of combustion. So that is your enthalpy of reaction or combustion whatever you call it that is product absolute enthalpy minus reactants, so this will be the amount that you get.

(Refer Slide Time: 27:55)

1: Combustion & Thermochemistry

$$\Delta h_R \left(\frac{\text{kJ}}{\text{kg}_{\text{fuel}}} \right) = \frac{\Delta H_R}{\text{MW}_{\text{fuel}}} \quad \dots (1.32)$$

$$\Delta h_R \left(\frac{\text{kJ}}{\text{kg}_{\text{fuel}}} \right) = \left(\frac{-802,405}{16.003} \right)$$

$$= -50,016$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR
Ashoke De 95

So, you can adjust this value to the per unit mass of the fuel. So one can write:

$$\Delta h_R / m_f = \Delta H_R / \text{MW}_{\text{fuel}}$$

So that you can get or you can write Δh_R which is per unit mass of fuel equals to:

$$\Delta h_R = -802405 / 16.003$$

So this would be 50.016. So that is how you can calculate it. So we will stop here and will continue in the next lecture. Thank you.