Turbulent Combustion: Theory and Modelling

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Lecture – 13

Heat and Mass Transfer (Contd.,) and Coupling of Chemical Kinetics and Thermodynamics

Welcome back. Let us continue the discussion on heat and mass transfer. So, what we look at the diffusion coefficient and from kinetic theory how we can get those coefficients. Now we look at some of the application of the mass transfer.

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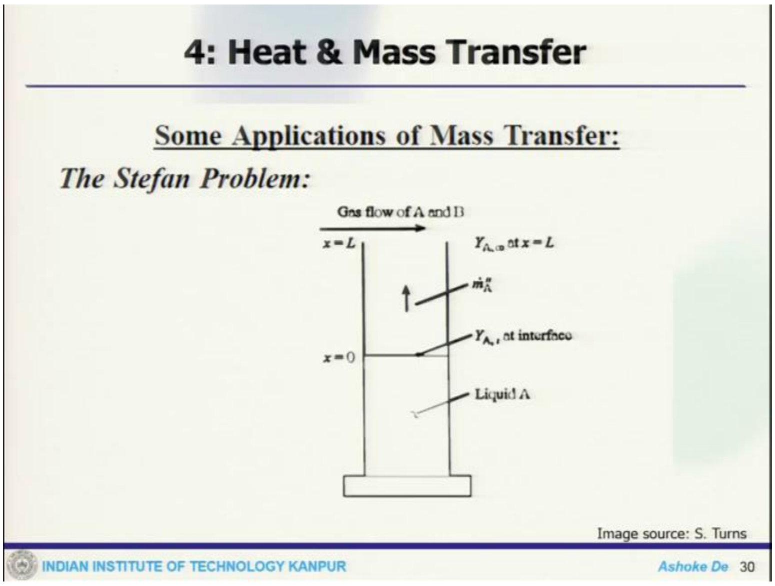

4: Heat & Mass Transfer

Some Applications of Mass Transfer:

The Stefan Problem:

Image source: S. Turns

For example we start the application of mass transfer. We look at this problem of Stefan problem. So here is a schematic of that particular one, through top there is a gas flow and that has A and B. And this is at coordinated at zero and this is A, and there are some other interface volume and this is liquid so that is the definition of the problem.

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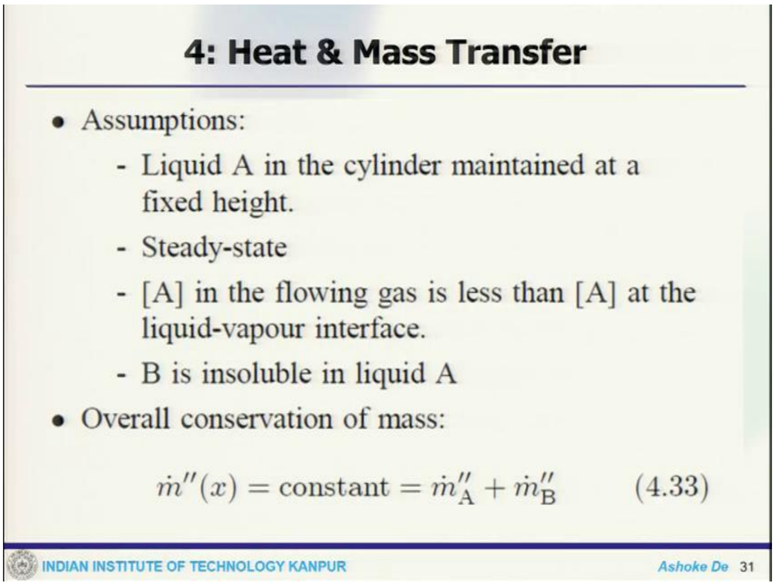

4: Heat & Mass Transfer

- Assumptions:
  - Liquid A in the cylinder maintained at a fixed height.
  - Steady-state
  - [A] in the flowing gas is less than [A] at the liquid-vapour interface.
  - B is insoluble in liquid A
- Overall conservation of mass:

$$\dot{m}''(x) = \text{constant} = \dot{m}''_{\mathrm{A}} + \dot{m}''_{\mathrm{B}} \qquad (4.33)$$

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Now there are some assumptions which are associated with Stefan problem. First one is the liquid A in the cylinder maintained at fixed height. So that means this is the liquid that is why this is the boundary condition that interferes this would be volume. So, within that this is maintained at fixed height. The whole thing is at steady-state, which is very, very important. Because once we assume steady-state then the equations with stands with them this disappears.

Then concentration A in the following flowing gas is less than A at the liquid vapour interface. So, this is the liquid vapour interface, so this so this is the interface. Now what it is that concentration of A in the flowing gas is less than that in the interface and B is insoluble in liquid A. Now, one can write the overall conservation of mass that is:

$$\dot{m}''(x) = constant = \dot{m}''_A + \dot{m}''_B$$

So, that is your sort of mass communication, which is one of the basic fundamental principal.

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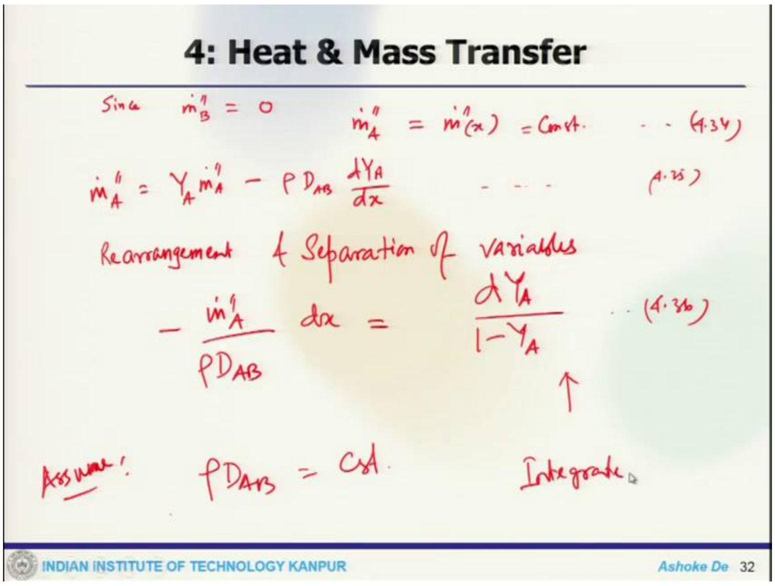

4: Heat & Mass Transfer

Since $\dot{m}''_B = 0$ $\quad \dot{m}''_A = \dot{m}''(x) = \text{Const.}$ . . (4.34)

$\dot{m}''_A = Y_A \dot{m}''_A - \rho D_{AB} \frac{dY_A}{dx}$ . . . . (4.35)

Rearrangement & Separation of variables

$- \frac{\dot{m}''_A}{\rho D_{AB}} dx = \frac{dY_A}{1-Y_A}$ . . (4.36)

↑

Integrate

Assume: $\rho D_{AB} = \text{Cst.}$

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Now since your $\dot{m}''_B$ is zero, $\dot{m}''_A$ becomes constant. Now we have already seen that:

$$\dot{m}''_A = Y_A \dot{m}''_A - \rho D_{AB} \frac{dY_A}{dx}$$

This is already established. Now, these three if we rearrange and separate the variables so what do you do? You do rearrangement and separation of variables so what we get?

$$- \frac{\dot{m}''_A}{\rho D_{AB}} dx = \frac{dY_A}{1 - Y_A}$$

So, that is what we get. Now if we assume ρD_{AB} to be constant, so that is one more assumption. If that is constant, then we can integrate this equation. So we can integrate and what we get.

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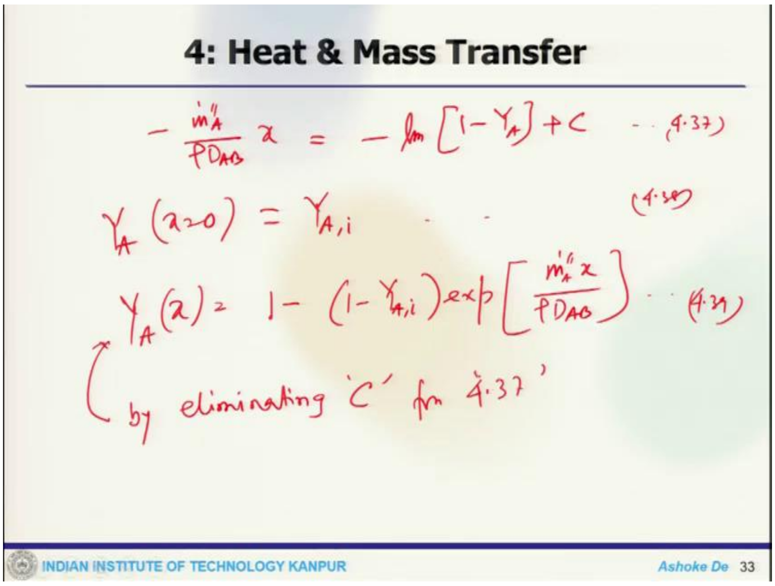

4: Heat & Mass Transfer

$- \frac{\dot{m}''_A}{\rho D_{AB}} x = - \ln [1 - Y_A] + C$ . . (4.37)

$Y_A (x=0) = Y_{A,i}$ . . (4.38)

$Y_A(x) = 1 - (1 - Y_{A,i}) \exp \left[\frac{\dot{m}''_A x}{\rho D_{AB}} \right]$ . . (4.39)

(by eliminating 'C' from 4.37)

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Then:

$$-\frac{\dot{m}''_A}{\rho D_{AB}}x = -ln[1 - Y_A] + C$$

So with the boundary condition so:

$$Y_A(x = 0) = Y_{A,i}$$

So using that, we can eliminate C so you get this boundary condition and then we get that:

$$Y_A(x) = 1 - (1 - Y_{A,i})exp\left[\frac{\dot{m}''_A x}{\rho D_{AB}}\right]$$

So that is what we get. This is by eliminating C that indication constant form 4.37. So that is what you get.

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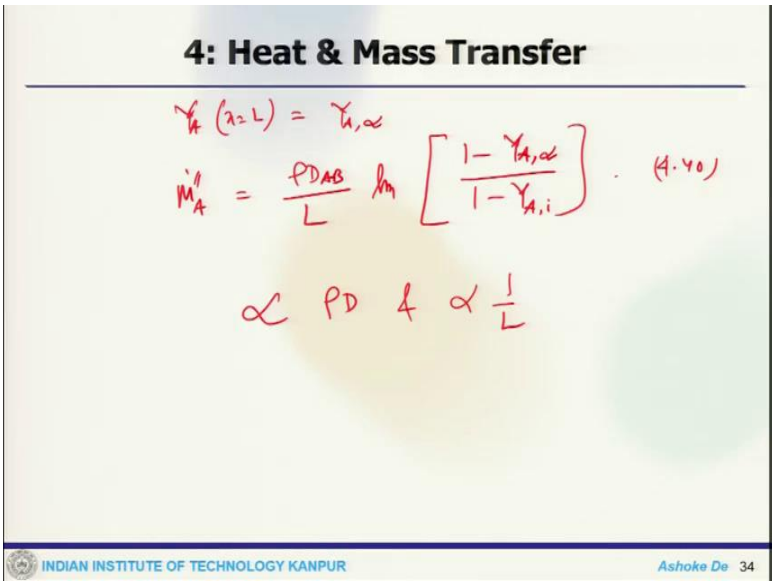

4: Heat & Mass Transfer

$$Y_A(x=L) = Y_{A,\infty}$$

$$\dot{m}''_A = \frac{\rho D_{AB}}{L} ln\left[\frac{1-Y_{A,\infty}}{1-Y_{A,i}}\right] . \quad (4.40)$$

$$\propto \rho D \ \& \ \propto \frac{1}{L}$$

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Now the mass flux of A for that we need one more boundary condition and that we can put at:

$$Y_A(x = L) = Y_{A,\infty}$$

So, once you put this in previous equation we get:

$$\dot{m}''_A = \frac{\rho D_{AB}}{L} ln\left[\frac{1 - Y_{A,\infty}}{1 - Y_{A,i}}\right]$$

Which is 4.40. This clearly shows you that is mass flux is proportional to ρD and inversely proportional to L. So, this is what we get regarding the mass flux.

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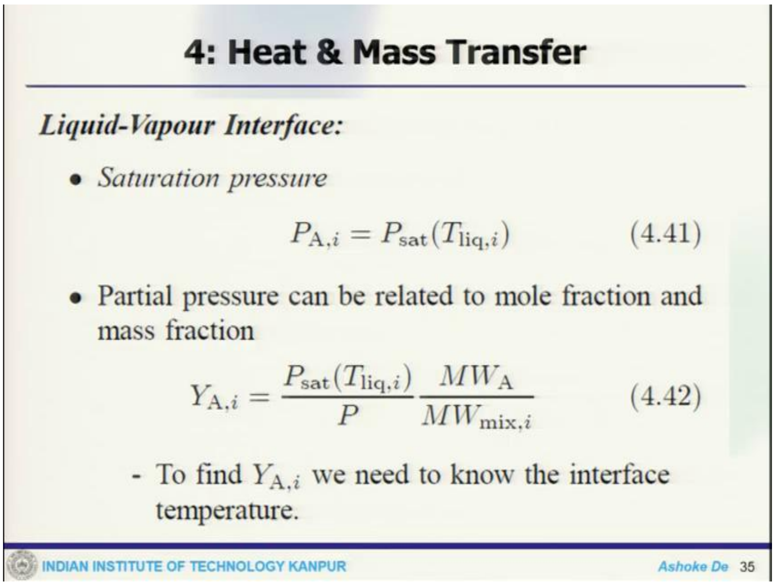

4: Heat & Mass Transfer

Liquid-Vapour Interface:

- *Saturation pressure*

$$P_{A,i} = P_{sat}(T_{liq,i}) \qquad (4.41)$$

- Partial pressure can be related to mole fraction and mass fraction

$$Y_{A,i} = \frac{P_{sat}(T_{liq,i})}{P} \frac{MW_A}{MW_{mix,i}} \qquad (4.42)$$

  - To find $Y_{A,i}$ we need to know the interface temperature.

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Now what happens at the liquid Vapour interface? So we need to look at that, because that is in situation were both liquid and vapour are there. So one is that saturation pressure so $P_{A,i}$would be saturation pressure of that liquid. Now we can correlate the partial pressure to mole fraction and mass fraction. So, mass fraction $Y_{A,i}$ would be:

$$Y_{A,i} = \frac{P_{sat}(T_{liq,i})}{P} . \frac{MW_A}{MW_{mix,i}}$$

So to find out this guy $Y_{A,i}$ we need to know the interface temperature. So, for that we need some boundary to condition.

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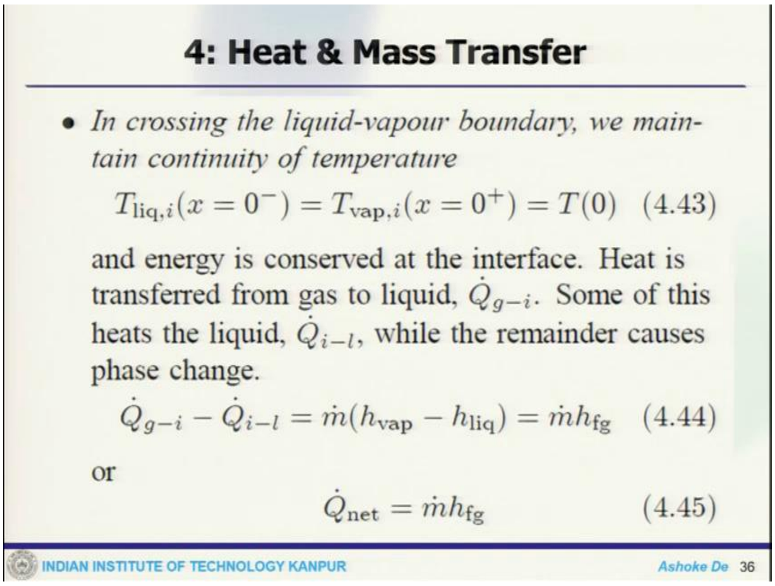

4: Heat & Mass Transfer

- *In crossing the liquid-vapour boundary, we maintain continuity of temperature*

$$T_{liq,i}(x = 0^-) = T_{vap,i}(x = 0^+) = T(0) \quad (4.43)$$

and energy is conserved at the interface. Heat is transferred from gas to liquid, $\dot{Q}_{g-i}$. Some of this heats the liquid, $\dot{Q}_{i-l}$, while the remainder causes phase change.

$$\dot{Q}_{g-i} - \dot{Q}_{i-l} = \dot{m}(h_{vap} - h_{liq}) = \dot{m}h_{fg} \quad (4.44)$$

or

$$\dot{Q}_{net} = \dot{m}h_{fg} \qquad (4.45)$$

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Now crossing the liquid vapour boundary, so, look at the continuity of the temperature. So, this is the temperature of the liquid at $x=0^-$ would be temperature of the vapour at 0^+ is T(0). So this is what we get and also at that point that means that interface point which you talk about this is the interface point that we are talking. So, energy is conserved at the interface. So heat transfer so this is the situation. This is the interface. This is vapour. This is liquid.

So that heat transferred from the gas to the liquid that is $\dot{Q}_{g-i}$ some of heats this liquid that go to liquid and rise to basically used to get the phase change. So,

$$\dot{Q}_{g-i} - \dot{Q}_{i-l} = \dot{m}\left(h_{vap} - h_{liq}\right) = \dot{m}h_{fg}$$

So, one can find out that $\dot{Q}_{net}$ is nothing but that change in enthalpy with mass loaded of that interface.

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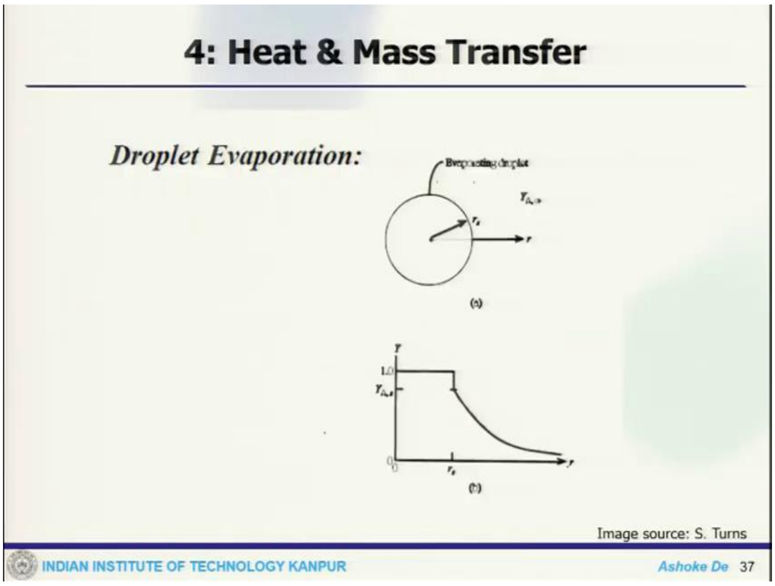

4: Heat & Mass Transfer

Droplet Evaporation:

Image source: S. Turns

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So, if there are droplets and that interface how that evaporate. So this is the evaporating droplet. This is in the radial direction and this is surface radius r_s and this y is infinity and this is how y and r will vary. So, they would be some assumption associated with that.

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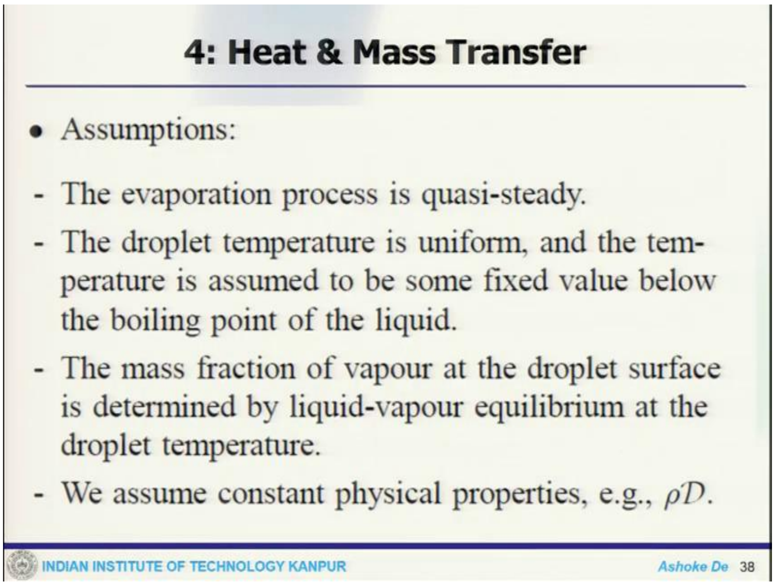

4: Heat & Mass Transfer

- Assumptions:
  - The evaporation process is quasi-steady.
  - The droplet temperature is uniform, and the temperature is assumed to be some fixed value below the boiling point of the liquid.
  - The mass fraction of vapour at the droplet surface is determined by liquid-vapour equilibrium at the droplet temperature.
  - We assume constant physical properties, e.g., ρD.

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The first assumption is that the evaporation process is quasi-steady is number one. When the droplet temperature is uniform and the temperature is assumed to be some fixed value below the boiling point of the liquid. So that is another important point then the mass fraction of vapour at the droplet interface is determined by liquid vapour equilibrium at the droplet temperature. And also we assume the constant physical properties like ρD like that.

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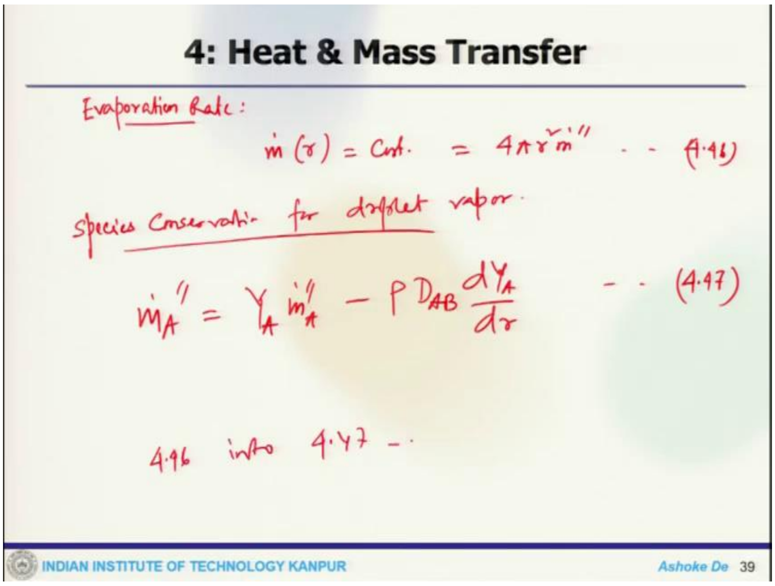

4: Heat & Mass Transfer

Evaporation Rate:

$$\dot{m}(r) = Const. = 4\pi r^2 \dot{m}'' \quad - - (4.46)$$

Species Conservation for droplet vapor.

$$\dot{m}_A'' = Y_A \dot{m}_A'' - \rho D_{AB} \frac{dY_A}{dr} \quad - - (4.47)$$

4.46 into 4.47 - -

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With these assumptions, one can find out the evaporation rate, it will be similar to the problem except change in coordinate system. So, overall mass conservation will give us:

$$\dot{m}(r) = constant = 4\pi r^2 \dot{m}''$$

So, that is my mass conservation. Then the species conservation for droplet vapour that would be another thing equals to:

$$\dot{m}''_A = Y_A \dot{m}''_A - \rho D_{AB} \frac{dY_A}{dr}$$

Which is 4.47.

So these are, one is the mass conservation and one is the species conservation. Now we substitute 4.46 into 4.47 and what we get.

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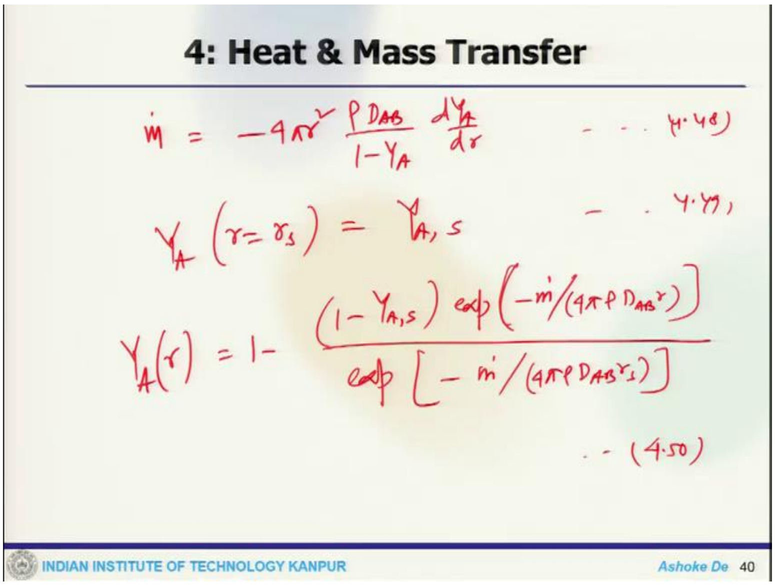

4: Heat & Mass Transfer

$$\dot{m} = -4\pi r^2 \frac{\rho D_{AB}}{1-Y_A} \frac{dY_A}{dr} \quad \text{- - . } (4.48)$$

$$Y_A (r = r_s) = Y_{A,s} \quad \text{- . } 4.49,$$

$$Y_A(r) = 1 - \frac{(1-Y_{A,s}) \exp\left(-\dot{m}/(4\pi\rho D_{AB} r)\right)}{\exp\left[-\dot{m}/(4\pi\rho D_{AB} r_s)\right]}$$

. - (4.50)

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We get results:

$$\dot{m} = 4\pi r^2 \frac{\rho D_{AB}}{1 - Y_A} \frac{dY_A}{dr}$$

Now once you get this you can always integrate and apply the boundary condition. So one of the boundary condition is that:

$$Y_A(r = r_s) = Y_{A,s}$$

Which will get you:

$$Y_A(r) = 1 - \frac{(1 - Y_{A,s}) exp\left(-\dot{m}/4\pi\rho D_{AB} r\right)}{exp\left(-\dot{m}/4\pi\rho D_{AB} r_s\right)}$$

So that is what you will get for radial profile of the mass fraction.

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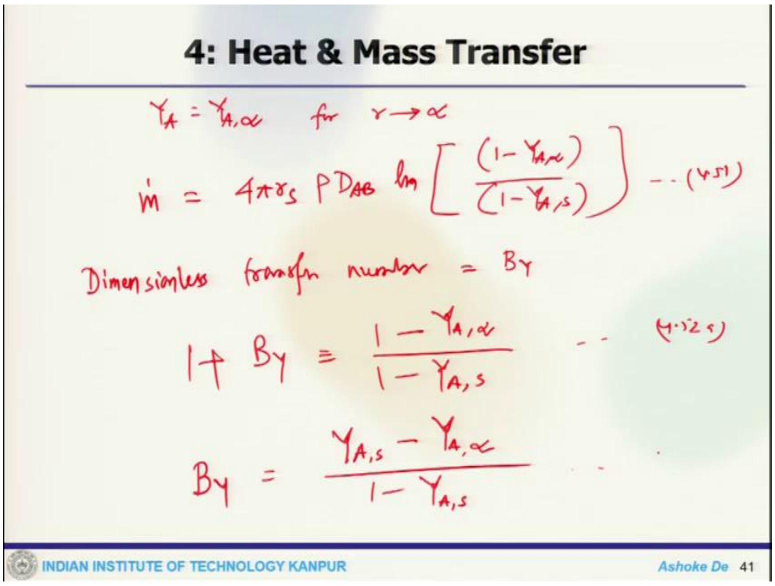

4: Heat & Mass Transfer

$Y_A = Y_{A,\infty}$ for $r \to \infty$

$$\dot{m} = 4\pi r_s \rho D_{AB} \ln\left[\frac{(1-Y_{A,\infty})}{(1-Y_{A,s})}\right] \quad \text{-- (4.51)}$$

Dimensionless transfer number $= B_Y$

$$1 + B_Y = \frac{1-Y_{A,\infty}}{1-Y_{A,s}} \quad \text{-- (4.52)}$$

$$B_Y = \frac{Y_{A,s}-Y_{A,\infty}}{1-Y_{A,s}}$$

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Now, we can calculate your operation rate from equation 4.50. By setting Y_A equals to $Y_{A,\infty}$ for r tends Infinity. So, then we can get:

$$\dot{m} = 4\pi r_s \rho D_{AB} ln\left[\frac{(1-Y_{A,\infty})}{(1-Y_{A,s})}\right]$$

So in this equation, one can define the dimensionless transfer number. So the dimensionless transfer number which is let us say B_y then:

$$1 + B_y = \frac{(1-Y_{A,\infty})}{(1-Y_{A,s})}$$

Once we define this dimensional number we actually can write it in a slightly different form:

$$B_y = \frac{(Y_{A,s}-Y_{A,\infty})}{(1-Y_{A,s})}$$

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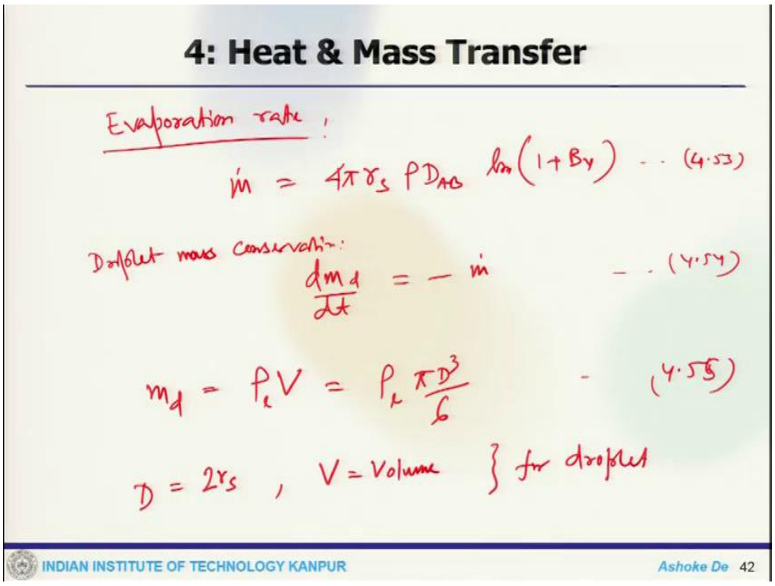

4: Heat & Mass Transfer

Evaporation rate:

$$\dot{m} = 4\pi r_s \rho D_{AB} \ln(1+B_y) \quad \ldots (4.53)$$

Droplet mass conservation:

$$\frac{dm_d}{dt} = -\dot{m} \quad \ldots (4.54)$$

$$m_d = \rho_l V = \rho_l \frac{\pi D^3}{6} \quad - (4.55)$$

$D = 2r_s$, V = Volume } for droplet

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So, we will lead to calculate the evaporation rate, so, the evaporation rate one can find out which will get you:

$$\dot{m} = 4\pi r_s \rho D_{AB} ln(1 + B_y)$$

Now droplet mass conservation so that is also another thing. So, to look at that droplet mass conservation we get:

$$\frac{dm_d}{dt} = -\dot{m}$$

So, that is how you get:

$$m_d = \rho_l V = \rho_l \frac{\pi D^3}{6}$$

That is 4.55. So, that is what you get. And here D is the diameter, V is the volume these are for that droplet.

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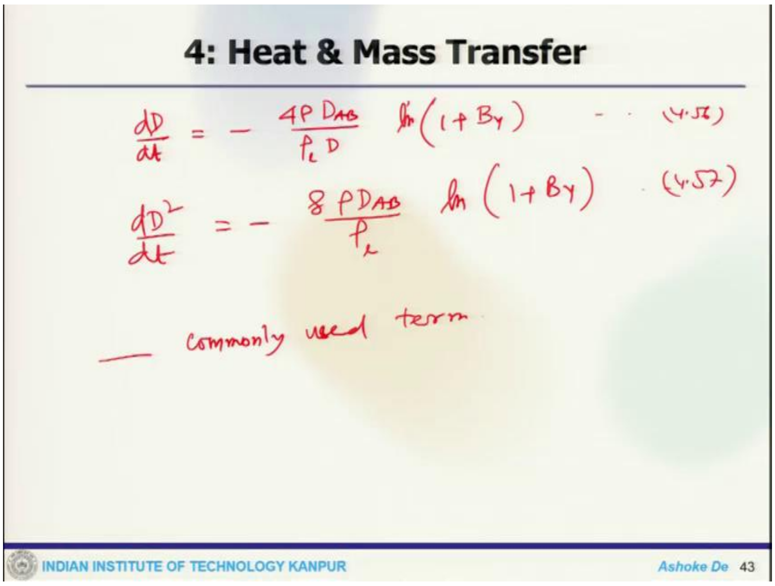

4: Heat & Mass Transfer

$$\frac{dD}{dt} = -\frac{4\rho D_{AB}}{\rho_l D} \ln(1+B_Y) \quad \cdots (4.56)$$

$$\frac{dD^2}{dt} = -\frac{8\rho D_{AB}}{\rho_l} \ln(1+B_Y) \quad . (4.57)$$

— commonly used term.

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Now once we get this substitute this 4.55 and 4.53 into 54 and differentiating you get:

$$\frac{dD}{dt} = -\frac{4\rho D_{AB}}{\rho_l D} ln(1+B_y)$$

So this is more commonly expressed in terms of the square and then D. So if you take the $\left(\frac{dD^2}{dt}\right)$ this will be:

$$\frac{dD^2}{dt} = -\frac{8\rho D_{AB}}{\rho_l D} ln(1+B_y)$$

So, it will tell us the time derivative of the square of the droplets. So this is quite commonly used term. And it tells us that the derivative of the square of the droplet diameter is constant.

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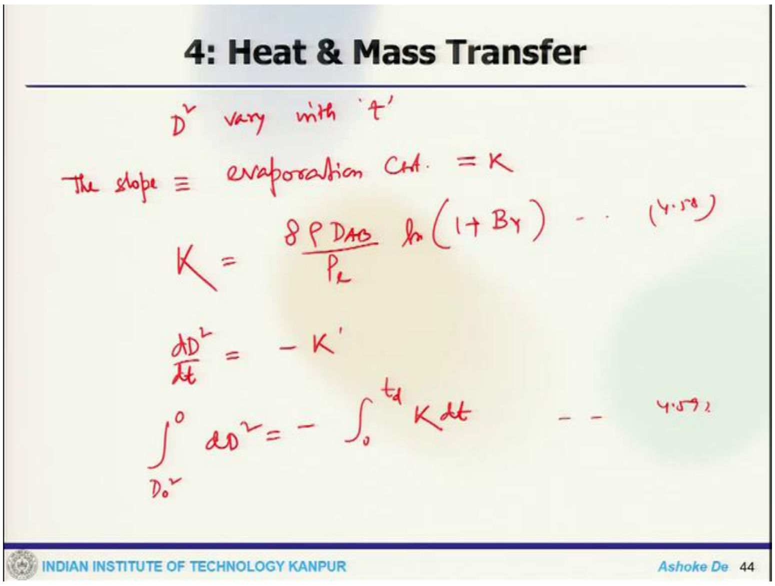

4: Heat & Mass Transfer

D^2 vary with 't'

The slope ≡ evaporation Cst. = K

$$K = \frac{8\rho D_{AB}}{\rho_l} \ln(1+B_Y) \quad \cdots (4.58)$$

$$\frac{dD^2}{dt} = -K$$

$$\int_{D_0^2}^{0} dD^2 = -\int_0^{t_d} K\,dt \quad -- \; 4.59)$$

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So, D^2 vary with t time which is the slope that is equal to the right hand side of this particular equation. And that slope would be and essentially the slope is the evaporation constant which is K and that K is:

$$K = \frac{8\rho D_{AB}}{\rho_l D} ln\left(1 + B_y\right)$$

Once you have this, one can find out the droplet evaporation time. So, essentially if you look at the previous expression, so that boils down to:

$$\frac{dD^2}{dt} = -K$$

Now if you integrate this, this would be:

$$\int_{D_0^2}^{0} dD^2 = -\int_{0}^{t_d} K\, dt$$

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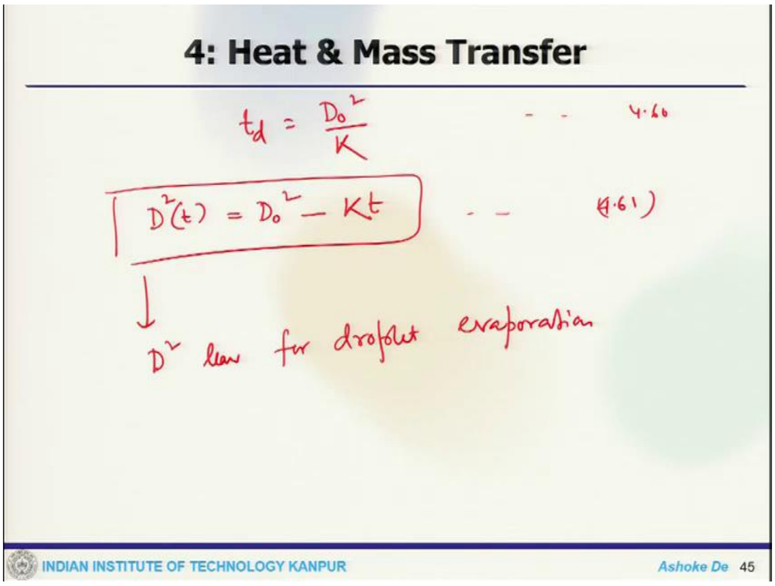

4: Heat & Mass Transfer

$t_d = \frac{D_0^2}{K}$ -- 4.60

$\boxed{D^2(t) = D_0^2 - Kt}$ -- (4.61)

$\downarrow$

D^2 law for droplet evaporation

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Which will get you:

$$t_d = \frac{D_0^2}{K}$$

And if change the limit to get more general relationship to provide the general expression for the variation of the D. So this will get you:

$$D^2(t) = D_0^2 - Kt$$

This is more generic expression. And this is commonly known as referred as this one D^2 law for droplet evaporation which is two phase flow which is a very common or very well-known equation D^2 law.

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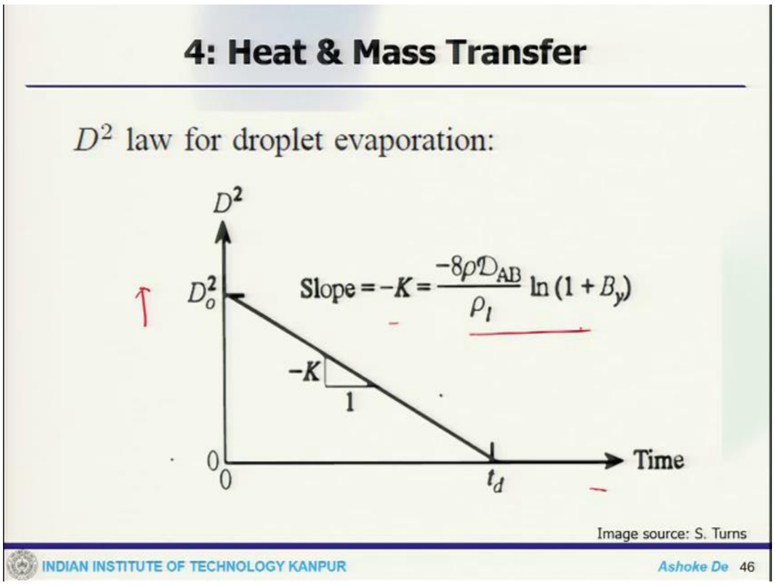

4: Heat & Mass Transfer

D^2 law for droplet evaporation:

Image source: S. Turns

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And what you see here is the D^2 law for droplet of evaporation, and that is the y axis and this is time and that is the slope, what do you get. So, this is well known D^2 law that you get. So, that is pretty much all about the Heat and mass transfer that we wanted to discuss.

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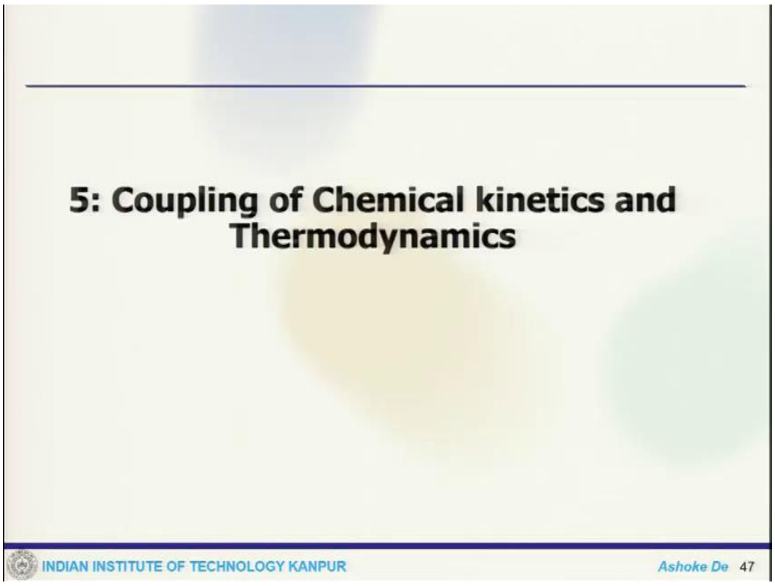

5: Coupling of Chemical kinetics and Thermodynamics

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And then will now move to the coupling of chemical kinetics under thermodynamics.

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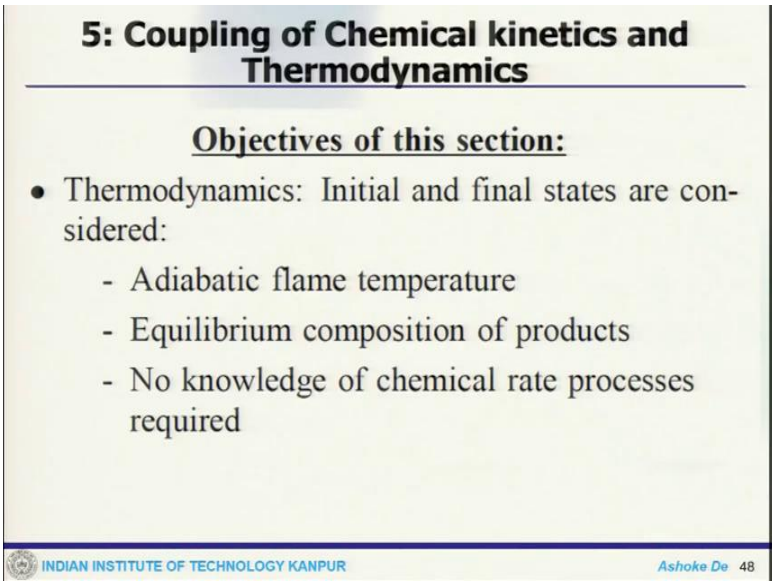

5: Coupling of Chemical kinetics and Thermodynamics

Objectives of this section:

- Thermodynamics: Initial and final states are considered:
  - Adiabatic flame temperature
  - Equilibrium composition of products
  - No knowledge of chemical rate processes required

So the idea of this is that we will now talk about some of the fundamental properties here like adiabatic flame temperature. So we talked but we never seen how we evaluate the adiabatic flame temperature. And then we can have equilibrium composition of the products that is also an important thing and then finally the knowledge of chemical rate processes, which is required.

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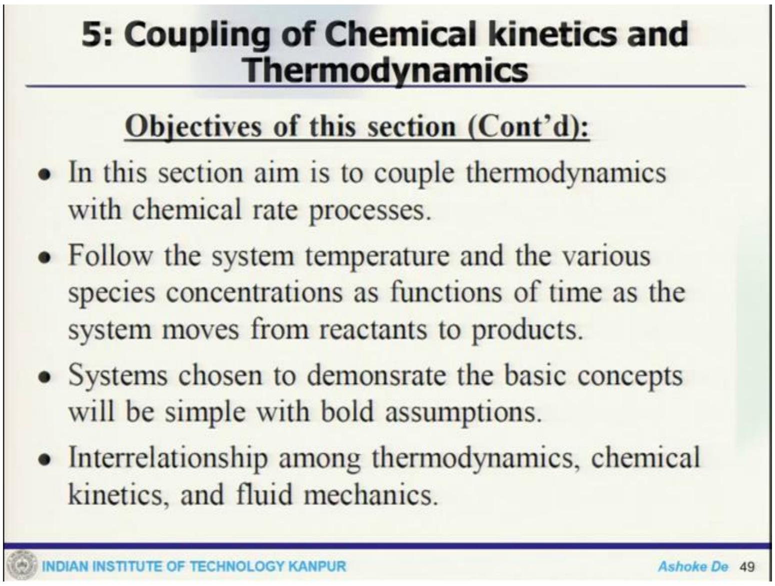

5: Coupling of Chemical kinetics and Thermodynamics

Objectives of this section (Cont'd):

- In this section aim is to couple thermodynamics with chemical rate processes.
- Follow the system temperature and the various species concentrations as functions of time as the system moves from reactants to products.
- Systems chosen to demonsrate the basic concepts will be simple with bold assumptions.
- Interrelationship among thermodynamics, chemical kinetics, and fluid mechanics.

So the whole idea is that how we coupled thermodynamics with the chemical process. Because we have looked at the kinetics, we have looked at Basics of the thermodynamics. Now, we want to couple that thing up so we can follow the system temperature and the various species concentration as a function of time and then we can see how system moves from reactants to products.

To do that, we can choose some simple system to deal with and then finally the inter-relationship among thermodynamics and kinetics and fluid mechanics that can be established. So, this is the whole idea of keep our discussion.

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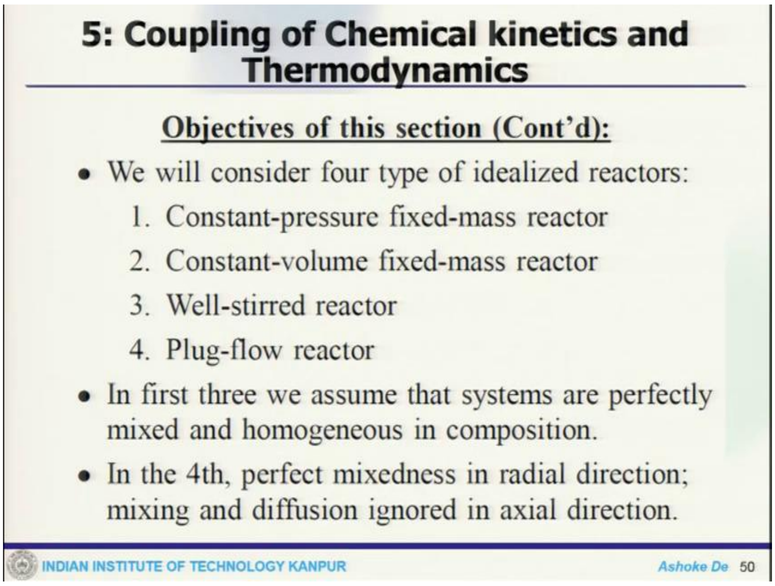

5: Coupling of Chemical kinetics and Thermodynamics

Objectives of this section (Cont'd):

- We will consider four type of idealized reactors:
  1. Constant-pressure fixed-mass reactor
  2. Constant-volume fixed-mass reactor
  3. Well-stirred reactor
  4. Plug-flow reactor
- In first three we assume that systems are perfectly mixed and homogeneous in composition.
- In the 4th, perfect mixedness in radial direction; mixing and diffusion ignored in axial direction.

Now to do that we will consider 4 types of idealized reactors, so, one is the constant pressure fixed mass reactor that is one thing that will consider first. So these are the simple idealistic situation which we will consider to demonstrate the coupling between kinetics and the thermodynamics. Then the constant volume fixed mass reactor and that is the second one and then we will continue the discussion.

Third will be well-stirred reactor and fourth one would be plug flow reactor. So, in this thing the first three here they are perfectly mix and homogeneous in composition. And the fourth perfect mix in radial direction and mixing and diffusion are ignored in the axial direction. So once we define the system that will actually tell us how.

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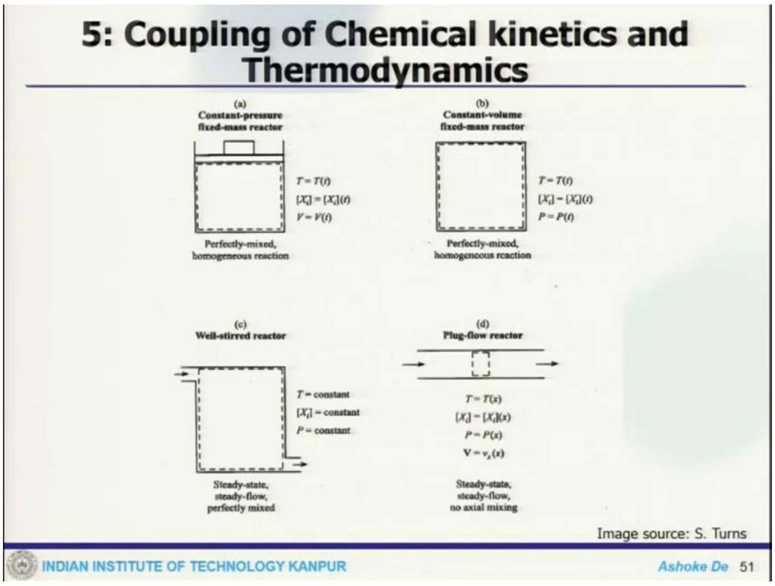

5: Coupling of Chemical kinetics and Thermodynamics

Image source: S. Turns

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Ashoke De 51

So this is the constant fixed mass reactor. Here, as we said the perfectly mixed homogeneous reaction. So, T will be function of time concentration will be the function of time, volume concentration of because it is constant pressure system. Now the second one is the constant volume, pressure will vary with time. Concentration varied time temperature in varied time. So, this is also perfectly mixed and homogeneous reaction which will take place here.

Third one well-stirred reactor some reactants comes in or goes out to temperature will be constant, pressure constant and concentration constant. And it is in steady-state steady flow perfectly mixed. Okay and fourth one is the plug flow reactor where the reactant comes in there is a control volume with the goes out to temperature is the function of direction concentration is a function of the direction and pressure is the function of direction. Well it is like that. So it is a steady-state steady flow no actual mixing. So these are the things.

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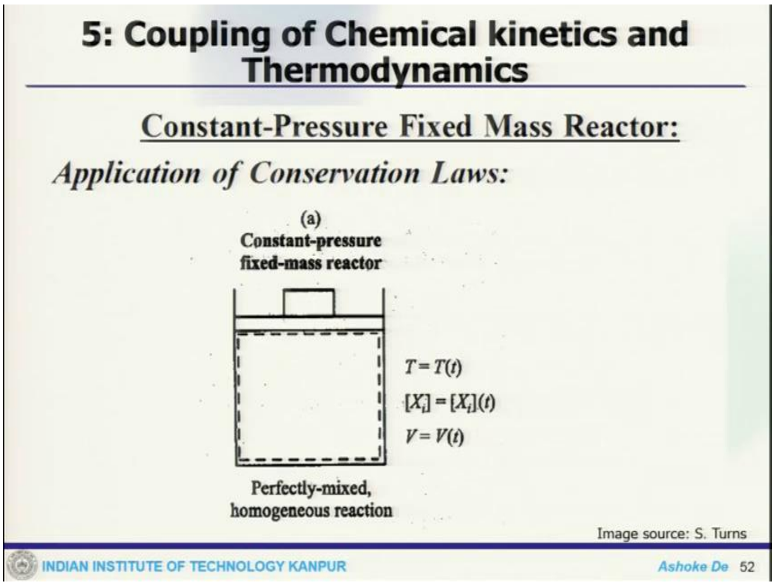

5: Coupling of Chemical kinetics and Thermodynamics

Constant-Pressure Fixed Mass Reactor:

Application of Conservation Laws:

Image source: S. Turns

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So now we first start with the constant pressure fixed mass reactor. So, the application of the conservation law to this perfectly mixed. So this is the schematic of that concentration and homogeneous reaction. What it does is the reactants reacts at each and every location within the volume at same time. So that is what it happens. So within this, the reactants react at each and every location of the volume.

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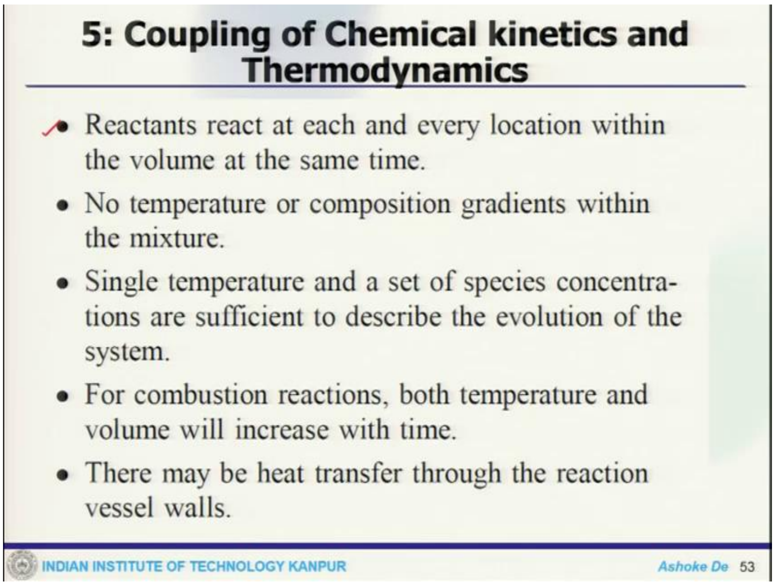

5: Coupling of Chemical kinetics and Thermodynamics

- Reactants react at each and every location within the volume at the same time.
- No temperature or composition gradients within the mixture.
- Single temperature and a set of species concentrations are sufficient to describe the evolution of the system.
- For combustion reactions, both temperature and volume will increase with time.
- There may be heat transfer through the reaction vessel walls.

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Ashoke De 53

Second no temperature composition gradient within the mixture that means within this there will be no temperature gradient or composition ingredient. Single temperature and state of species concentration are sufficient to describe the evolution of the system. See if we take this particular system that evolution can be described by a single temperature and certain species and now due to reaction both temperature and volume will increase with time. And there would be heat transfer to the reaction vessels so that is also going to be there.

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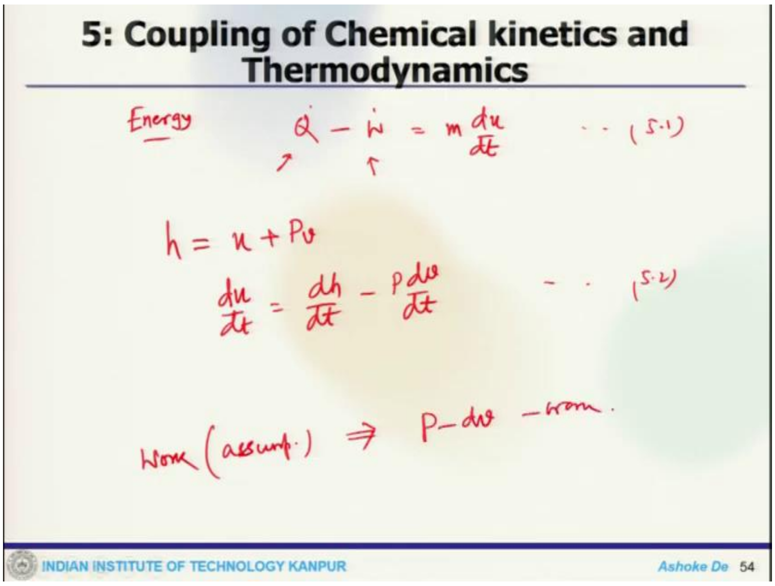

5: Coupling of Chemical kinetics and Thermodynamics

Energy $\dot{Q} - \dot{W} = m\frac{du}{dt}$ ... (5.1)

$h = u + Pv$

$\frac{du}{dt} = \frac{dh}{dt} - P\frac{dv}{dt}$ ... (5.2)

Work (assump.) ⇒ P-dv -work.

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Ashoke De 54

Now the conservation of energy for fixed mass system if we look at the energy conservation equation, so which will give us:

$$\dot{Q} - \dot{W} = m\frac{du}{dt}$$

Now $\dot{Q}$ is the heat transfer W is the work done. Now you use the definition of the enthalpy:

$$h = u + Pv$$

And differentiating will give us:

$$\frac{du}{dt} = \frac{dh}{dt} - P\frac{dv}{dt}$$

So, that is what we get. Now if we assume the work, so that is an assumption that is only the P-dv work at system.

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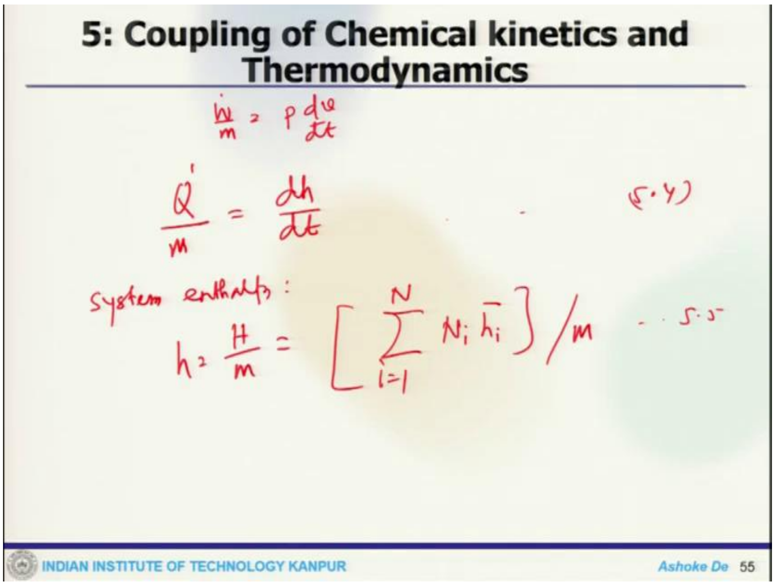

5: Coupling of Chemical kinetics and Thermodynamics

$$\frac{\dot{W}}{m} = P\frac{dv}{dt}$$

$$\frac{\dot{Q}}{m} = \frac{dh}{dt} \quad \ldots \quad (5.4)$$

System enthalpy:

$$h = \frac{H}{m} = \left[\sum_{i=1}^{N} N_i \bar{h}_i\right] / m \quad \ldots \; 5.5$$

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Ashoke De 55

And then:

$$\frac{\dot{W}}{m} = P\frac{dv}{dt}$$

And if you put things together what we get:

$$\frac{\dot{Q}}{m} = \frac{dh}{dt}$$

So that is what we get. Now the system enthalpy we can estimate in terms of composition so that will be:

$$h = \frac{H}{m} = {\left[\sum_{i=1}^{N} N_i \bar{h}_i\right]}\Big/_{m}$$

So you can calculate that these things.

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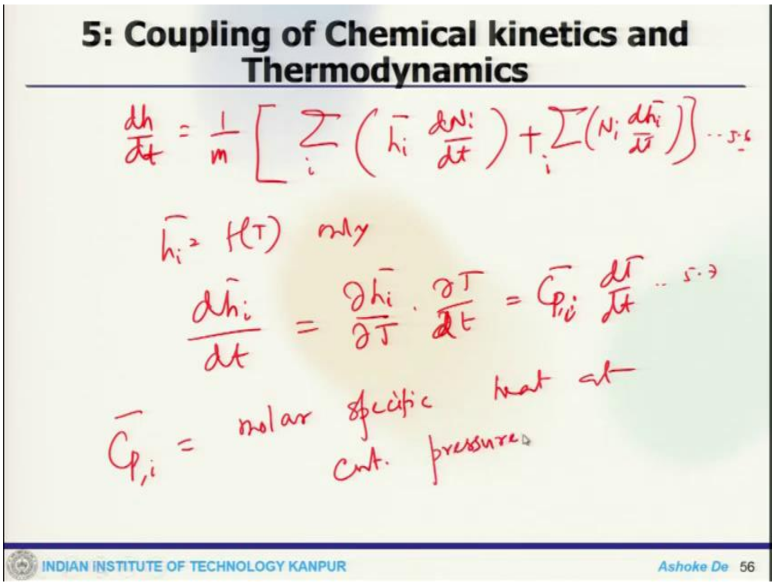

5: Coupling of Chemical kinetics and Thermodynamics

$$\frac{dh}{dt} = \frac{1}{m}\left[\sum_i \left(\bar{h}_i \frac{dN_i}{dt}\right) + \sum_i \left(N_i \frac{d\bar{h}_i}{dt}\right)\right] \quad ..5.6$$

$\bar{h}_i = f(T)$ only

$$\frac{d\bar{h}_i}{dt} = \frac{\partial \bar{h}_i}{\partial T}\cdot\frac{\partial T}{\partial t} = \bar{C}_{p,i}\frac{dT}{dt} \quad ..5.7$$

$\bar{C}_{p,i}$ = molar specific heat at cnt. pressure

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Now, we differentiating the previous equation gives you, once we differentiate that it will give you:

$$\frac{dh}{dt} = \frac{1}{m}\left[\sum_{i=1}^{N}\left(\bar{h}_\iota \frac{dN_i}{dt}\right) + \sum_{i=1}^{N}\left(N_i \frac{d\bar{h}_\iota}{dt}\right)\right]$$

So now $\bar{h}_\iota$ will be functional temperature only what one can is that:

$$\frac{d\bar{h}_\iota}{dt} = \frac{\partial \bar{h}_\iota}{\partial T}\frac{\partial T}{\partial t} = \bar{C}_{P,i}\frac{dT}{dt}$$

Now here $\bar{C}_{P,i}$ is a molar specific heat at constant pressure. So, this is where we stop today and pick it up in the next lecture.