Turbulent Combustion: Theory and Modelling
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Lecture – 14
Coupling of Chemical Kinetics and Thermodynamics (Contd.,)

Ok, welcome back. We were in the middle of the discussion of this coupling of kinetic and the Thermodynamics. And we started with some simple example and the one that we are discussing in the constant pressure fixed mass reactor and there would be few more that will take it up and look at this application.

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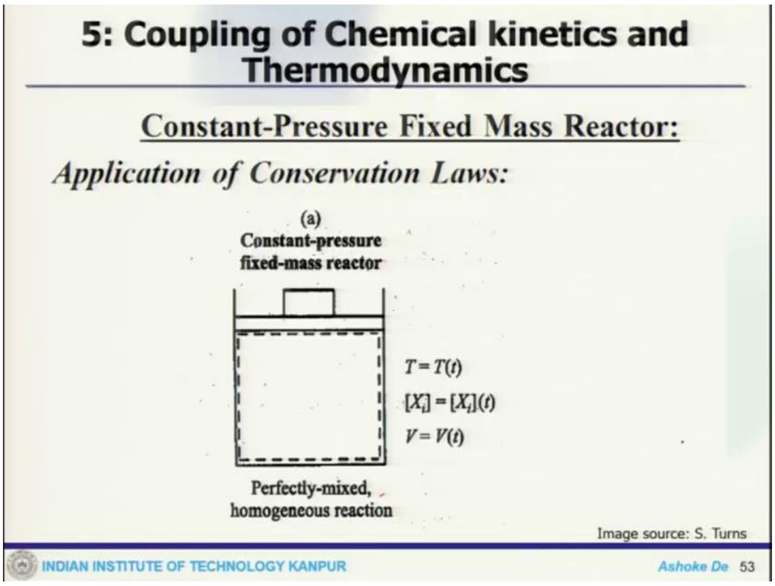

5: Coupling of Chemical kinetics and Thermodynamics

Constant-Pressure Fixed Mass Reactor:

Application of Conservation Laws:

Image source: S. Turns

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So this is where you are actively looking at it. This is a constant pressure fixed mass reactor. That was the schematic just to give you a quick refreshment where we stop.

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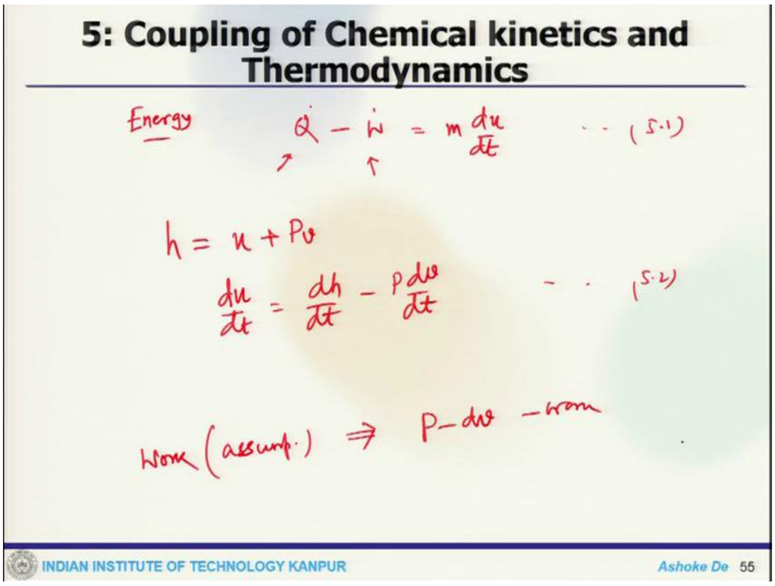

5: Coupling of Chemical kinetics and Thermodynamics

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.) $\Rightarrow$ P-dv -work

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And these are the assumption then we wrote our energy equation and then we got the enthalpy and then we have work. This is one of the biggest assumption is that work is only the P-dv work.

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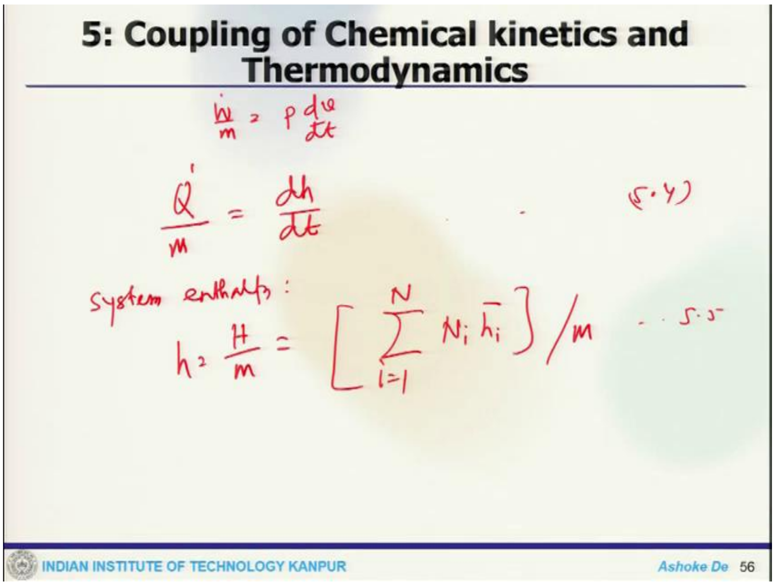

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$\frac{\dot{W}}{m} = P\frac{dv}{dt}$

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

System enthalpy:

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

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Then finally we replace that thing.

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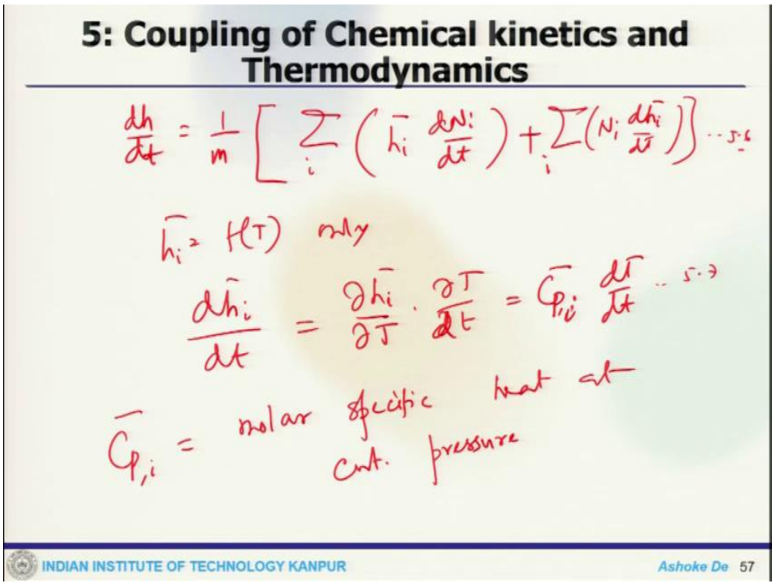

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$$\frac{dh}{dt} = \frac{1}{m}\left[\sum_i \left(\bar{h}_i \frac{dN_i}{dt}\right) + \sum_i \left(N_i \frac{d\bar{h}_i}{dt}\right)\right] \quad ..5.6$$

$\bar{h}_i = f(T)$ 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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And this is where we stopped the ideal gas behaviour. This is equation 5.7.

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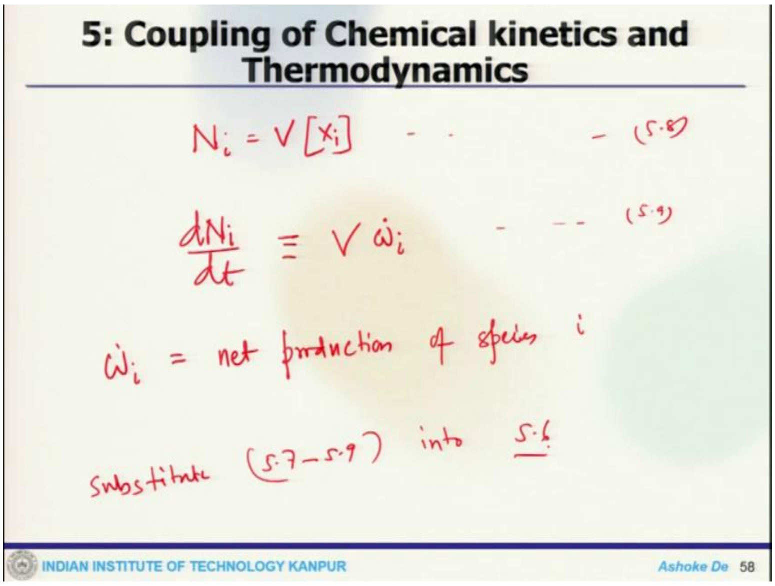

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$$N_i = V[X_i] \quad \text{-- (5.8)}$$

$$\frac{dN_i}{dt} \equiv V\dot{\omega}_i \quad \text{--- (5.9)}$$

$\dot{\omega}_i$ = net production of species i

substitute (5.7 – 5.9) into $\underline{5.6}$

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Now the 5.7 provide the link to the system temperature and the system composition they are linked with like this. So, this is 5.8 and now chemical dynamics that can be linked as:

$$\frac{dN_i}{dt} \equiv V\dot{\omega}_i$$

That is where my $\dot{\omega}_i$ is the net production of species i, so this already have seen it. Now if you to substitute this 5.7 in to 5.9. So, basically you want to substitute 5.7 to 5.9 into 5.6, once you do that what we get is that.

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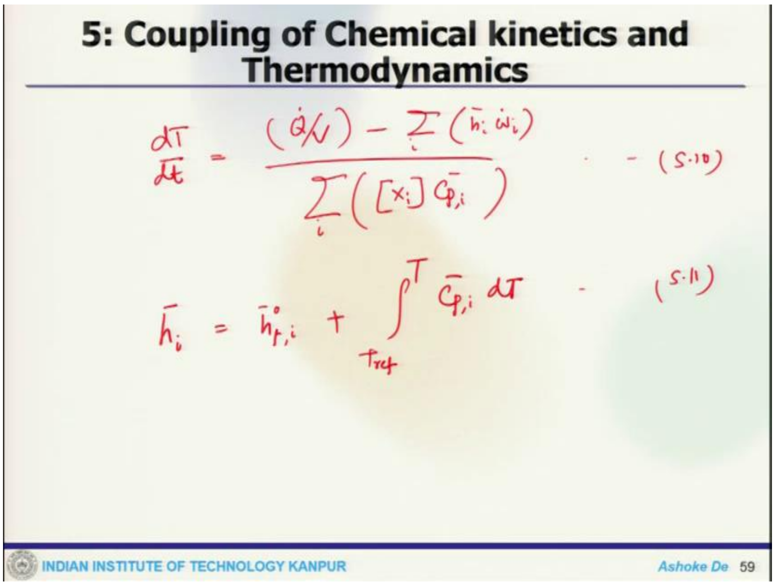

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$$\frac{dT}{dt} = \frac{(\dot{Q}/V) - \sum_i (\bar{h}_i \dot{\omega}_i)}{\sum_i ([X_i] \bar{C}_{P,i})} \qquad \text{- - (5.10)}$$

$$\bar{h}_i = \bar{h}^{\circ}_{f,i} + \int_{T_{ref}}^{T} \bar{C}_{P,i}\, dT \qquad \text{- (5.11)}$$

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$$\frac{dT}{dt} = \frac{\left(\dot{Q}/_V\right) - \sum_i (\bar{h}_\iota \dot{\omega}_\iota)}{\sum_i ([X_i] \bar{C}_{P,i})}$$

And this will take over all this is there. Now once we use the calorific equation of state which states that this is:

$$\bar{h}_\iota = \bar{h}_i^0 + \int_{T_{ref}}^{T} \bar{C}_{P,i}\, dT$$

So that what we get now, one can find out using this the volume so that can be easily obtained.

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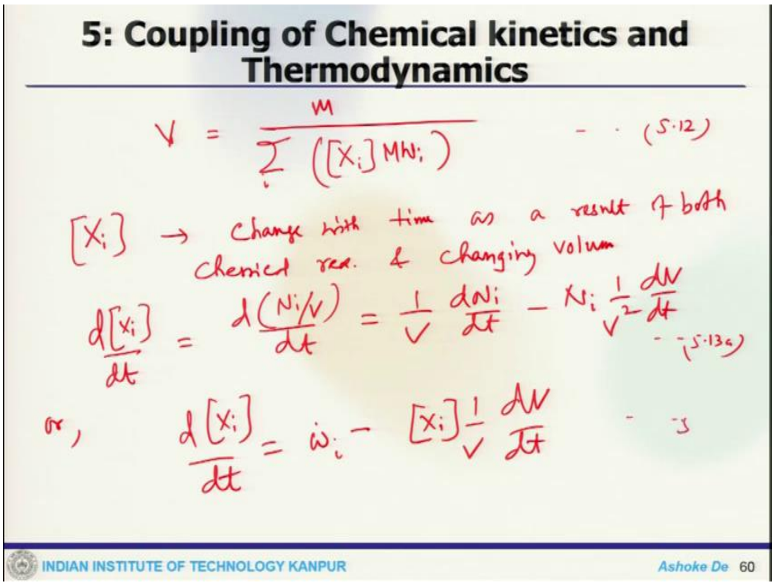

5: Coupling of Chemical kinetics and Thermodynamics

$$V = \frac{m}{\sum_i ([X_i] MW_i)} \qquad \text{- - (5.12)}$$

$[X_i]$ → Change with time as a result of both chemical rea. & changing volume

$$\frac{d[X_i]}{dt} = \frac{d(N_i/V)}{dt} = \frac{1}{V}\frac{dN_i}{dt} - N_i \frac{1}{V^2}\frac{dV}{dt} \qquad \text{- - (5.13a)}$$

$$\text{or,} \quad \frac{d[X_i]}{dt} = \dot{\omega}_i - [X_i]\frac{1}{V}\frac{dV}{dt} \qquad \text{- - 5}$$

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And the volume would be:

$$V = \frac{m}{\sum_i([X_i]MW_i)}$$

$[X_i]$ is concentration molecular weight of i which is; now this is the change with time as a result of both chemical reaction and changing volume. So, what one can write:

$$\frac{d[X_i]}{dt} = \frac{d\left(N_i/_V\right)}{dt} = \frac{1}{V}\frac{dN_i}{dt} - N_i\frac{1}{V^2}\frac{dV}{dt}$$

So, or one can write:

$$\frac{d[X_i]}{dt} = \dot{\omega}_i - [X_i]\frac{1}{V}\frac{dV}{dt}$$

That is my 13b.

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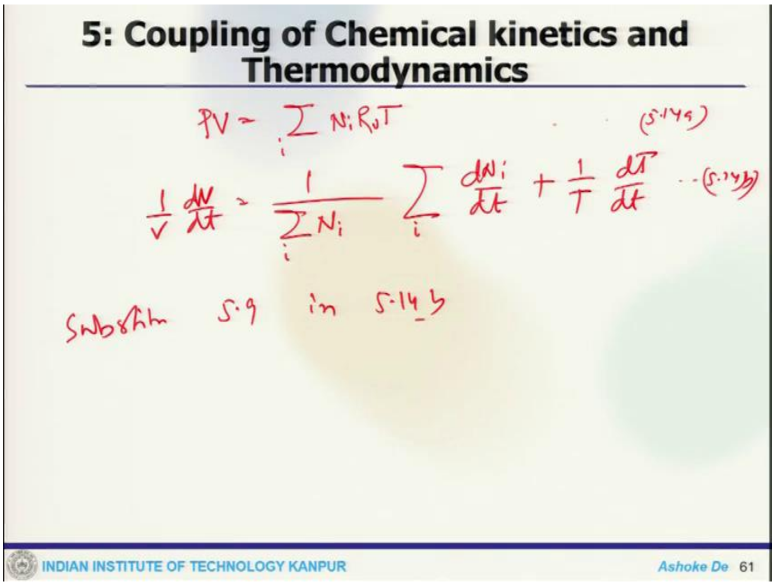

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$$PV = \sum_i N_i R_u T \qquad (5.14a)$$

$$\frac{1}{V}\frac{dV}{dt} = \frac{1}{\sum_i N_i}\sum_i \frac{dN_i}{dt} + \frac{1}{T}\frac{dT}{dt} \quad \cdots (5.14b)$$

Substitute 5.9 in 5.14b

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So again, we use the ideal gas law which is nothing but:

$$PV = \sum_i N_i R_u T$$

Now here P is constant. So if you differentiate this equation and rearrange that this will get:

$$\frac{1}{V}\frac{dV}{dt} = \frac{1}{\sum_i N_i}\sum_i \frac{dN_i}{dt} + \frac{1}{T}\frac{dT}{dt}$$

For this particular system pressure is constant. Now we substitute 5.9 into 5.14b and then you substitute the result of 5.13b.

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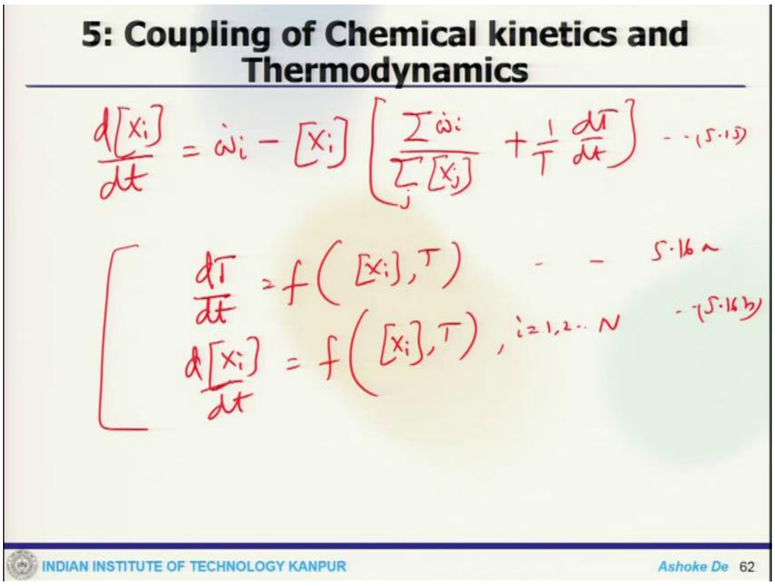

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$$\frac{d[X_i]}{dt} = \dot{\omega}_i - [X_i]\left[\frac{\sum \dot{\omega}_i}{\sum_j [X_j]} + \frac{1}{T}\frac{dT}{dt}\right] \quad - - (5.15)$$

$$\left[\begin{aligned} &\frac{dT}{dt} = f([X_i], T) &&- - \; 5.16\,a \\ &\frac{d[X_i]}{dt} = f([X_i], T), \; i = 1,2.. N &&- (5.16\,b) \end{aligned}\right.$$

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So that will get us:

$$\frac{d[X_i]}{dt} = \dot{\omega}_\iota - [X_i]\left[\frac{\sum \dot{\omega}_\iota}{\sum_j [X_j]} + \frac{1}{T}\frac{dT}{dt}\right]$$

In summary, the problem is to find out the solution of the following two set of differential equation 1 is that:

$$\frac{dT}{dt} = f([X_i], T)$$

And T that is number one and the second one would be this is a function of T. So, this is the bottom line to setup equation and the whole idea is to find out the solution of these two.

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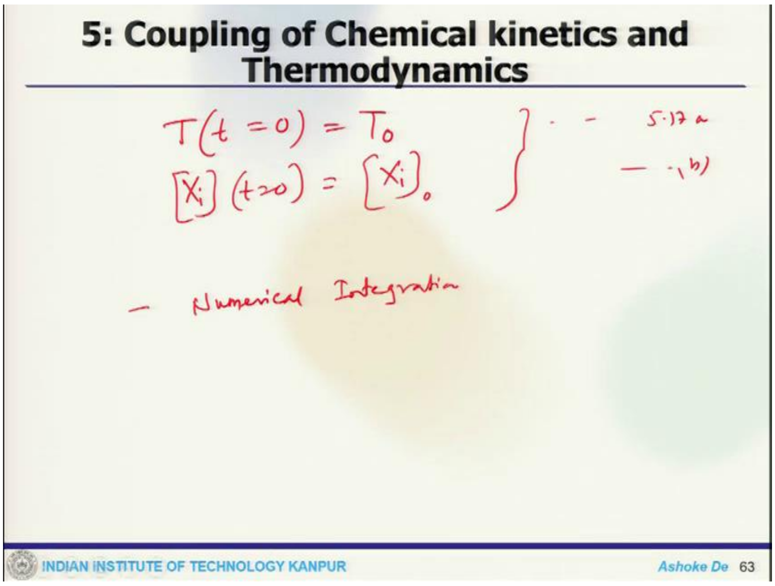

5: Coupling of Chemical kinetics and Thermodynamics

$$\left.\begin{aligned} &T(t=0) = T_0 \\ &[X_i](t=0) = [X_i]_0 \end{aligned}\right\} \quad \begin{aligned} &- - \; 5.17\,a \\ &- \; - (b) \end{aligned}$$

– Numerical Integration

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So, this equations are subjected to some initial conditions where t at 0 is T_0 and

$$[X_i](t = 0) = [X_i]_0$$

So this is a and this is b. Now this functional form of these two equations are obtained from equation 5.10 and 5.11 gives enthalpy and equation 5.1 to give volume. But what happens most of the time there is no analytical solution. So, one has to go by some numerical technique like numerical integration. And which is somehow capable of handling this strip system.

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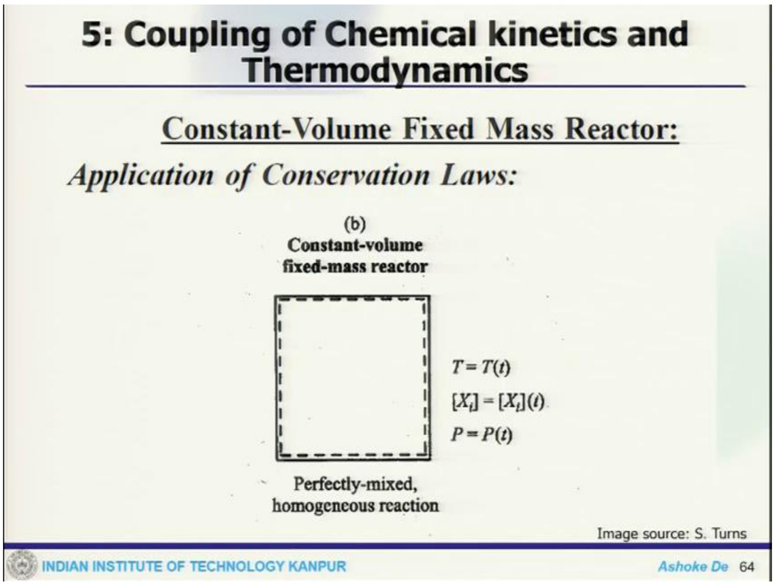

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Constant-Volume Fixed Mass Reactor:

Application of Conservation Laws:

(b)
Constant-volume fixed-mass reactor

$T = T(t)$
$[X_i] = [X_i](t)$
$P = P(t)$

Perfectly-mixed, homogeneous reaction

Image source: S. Turns

Now I will move to the next reactor which is a constant volume fixed mass reactor. So, this volume is fixed and things should only change with time. Now again this case also, Energy equation will apply which will be similar to constant pressure case.

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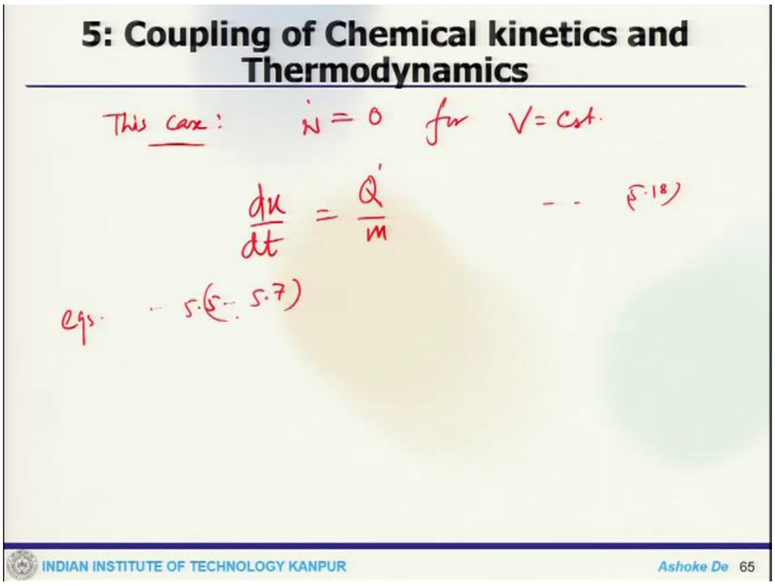

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This case: $\dot{\omega} = 0$ for $V = Cst.$

$$\frac{du}{dt} = \frac{\dot{Q}}{m} \quad \text{-- } 5.18)$$

eqs. -- 5.5 -- 5.7)

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And only exception here is that this particular case, so this case our $\dot{\omega}$ for constant V constant previously V was changing. So, there is a work done due to P/V work. So, my energy equation will get me:

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

Now u here plays the same role as h in our analysis for P constant. Now the equations or that we got from 5.5 to 5.7. So similar things can be developed here and can be used in this particular equation. So essentially this is one expression this is second expression this is third expressions all this would be applicable and we can use them up and put it in this particular equation.

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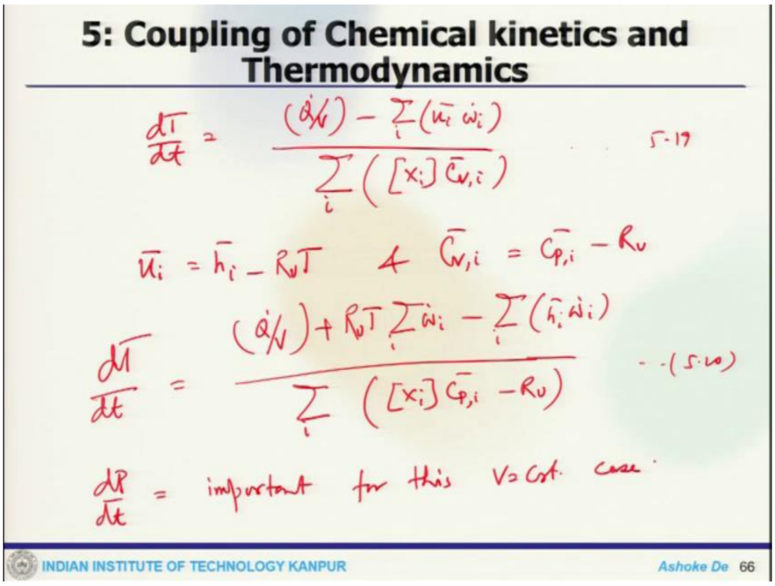

5: Coupling of Chemical kinetics and Thermodynamics

$$\frac{dT}{dt} = \frac{(\dot{Q}/V) - \sum_i (\bar{u}_i \dot{\omega}_i)}{\sum_i ([X_i] \bar{C}_{v,i})} \quad 5.19$$

$$\bar{u}_i = \bar{h}_i - R_u T \quad \& \quad \bar{C}_{v,i} = \bar{C}_{p,i} - R_u$$

$$\frac{dT}{dt} = \frac{(\dot{Q}/V) + R_u T \sum_i \dot{\omega}_i - \sum_i (\bar{h}_i \dot{\omega}_i)}{\sum_i ([X_i] \bar{C}_{p,i} - R_u)} \quad \text{--}(5.20)$$

$\frac{dP}{dt}$ = important for this V = Cst. case.

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To get that my $\left(\frac{dT}{dt}\right)$ would be:

$$\frac{dT}{dt} = \frac{\left(\dot{Q}/_{V}\right) - \sum_i(\bar{u}_i\dot{\omega}_i)}{\sum_i\left([X_i]\bar{C}_{v,i}\right)}$$

So that is my temperature. Now you have:

$$\bar{u}_i = \bar{h}_i - R_uT$$

And

$$\bar{C}_{v,i} = \bar{C}_{P,i} - R_u$$

So, once we put them back you get:

$$\frac{dT}{dt} = \frac{\left(\dot{Q}/_{V}\right) + R_uT\sum_i(\dot{\omega}_i) - \sum_i\left(\bar{h}_i\dot{\omega}_i\right)}{\sum_i\left([X_i]\bar{C}_{P,i} - R_u\right)}$$

So, this is what we get here $\left(\frac{dP}{dt}\right)$ is quite important this is important for this V equals to constant case. Because V constant case is the term disappeared. So in this case V should not disappear and that would be quite important.

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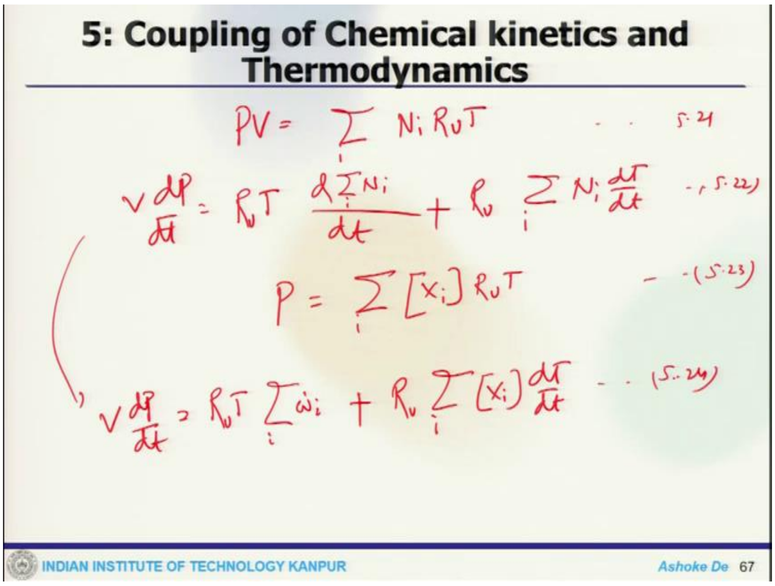

5: Coupling of Chemical kinetics and Thermodynamics

$$PV = \sum_i N_iR_uT \quad \cdots \; 5\cdot21$$

$$V\frac{dP}{dt} = R_uT\frac{d\sum_i N_i}{dt} + R_u\sum_i N_i\frac{dT}{dt} \quad \cdots\; 5\cdot22)$$

$$P = \sum_i [X_i]R_uT \quad - \cdot(5\cdot23)$$

$$V\frac{dP}{dt} = R_uT\sum_i\dot{\omega}_i + R_u\sum_i[X_i]\frac{dT}{dt} \quad \cdots\; (5\cdot24)$$

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Now to get $\left(\frac{dP}{dt}\right)$ again start using the ideal gas law which is:

$$PV = \sum_i N_iR_uT$$

And we get:

$$V\frac{dP}{dt} = R_uT\frac{d\sum_i N_i}{dt} + R_u\sum_i N_i\frac{dT}{dt}$$

So that is the total pressure of the system. From here we get:

$$V\frac{dP}{dt} = R_uT\sum_i \omega_i + R_u\sum_i [X_i]\frac{dT}{dt}$$

Now this 5.20 can be integrated.

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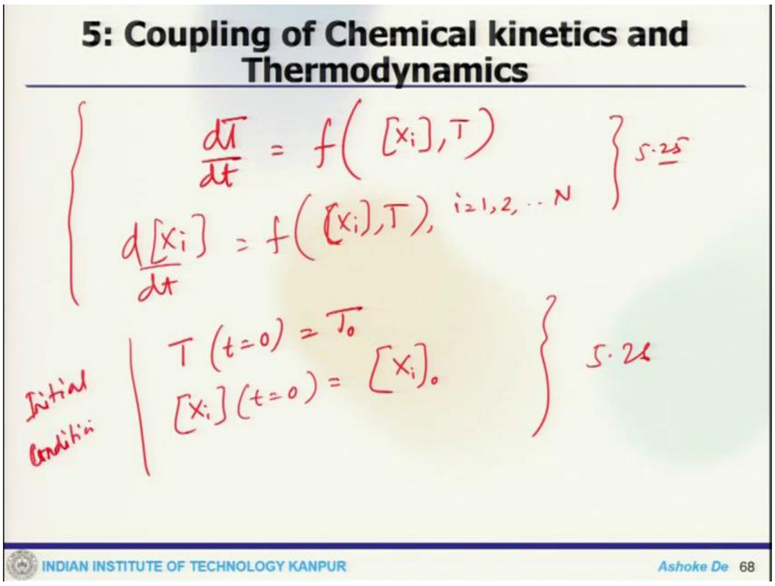

5: Coupling of Chemical kinetics and Thermodynamics

$$\left.\begin{aligned} \frac{dT}{dt} &= f([X_i],T) \\ \frac{d[X_i]}{dt} &= f([X_i],T), \quad i=1,2,..N \end{aligned}\right\} 5.25$$

Initial Condition

$$\left.\begin{aligned} T(t=0) &= T_0 \\ [X_i](t=0) &= [X_i]_0 \end{aligned}\right\} 5.26$$

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And simultaneously to determine t and dT so what we get:

$$\frac{dT}{dt} = f([X_i],T)$$

We get a function of this and T for i equals to 1,2 to such that N, now these set of equations. They can be sort with the initial conditions like T equals to T_0 and:

$$[X_i](t=0) = [X_i]_0$$

So, these are the initial conditions. So this set of equation can be solved subjected to this initial condition.

Now that is how you get the solution for the temperature and concentration in the volume constant reactor.

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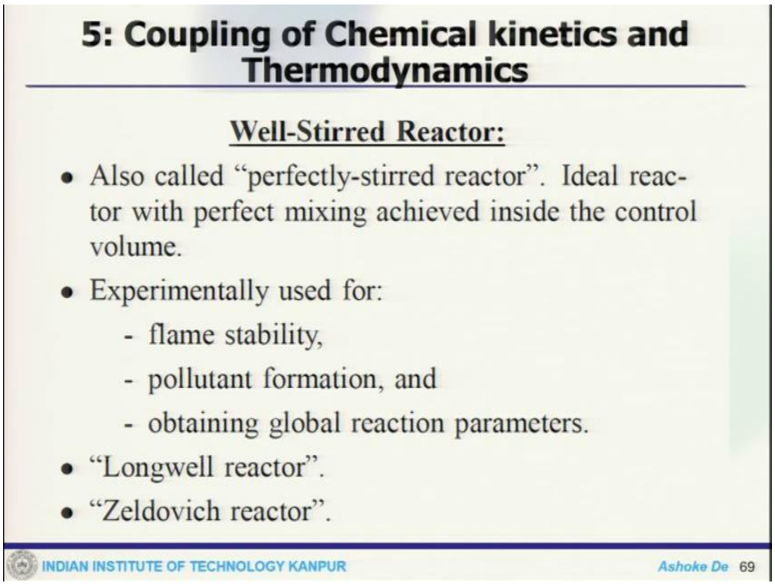

5: Coupling of Chemical kinetics and Thermodynamics

Well-Stirred Reactor:

- Also called "perfectly-stirred reactor". Ideal reactor with perfect mixing achieved inside the control volume.
- Experimentally used for:
  - flame stability,
  - pollutant formation, and
  - obtaining global reaction parameters.
- "Longwell reactor".
- "Zeldovich reactor".

Now you go to well stirred reactor, so the well stirred reactor is essentially the perfectly stirred reactor is ideal reactor with perfect mixing achieved inside the control volume. So, this is quite often used experimental setup for flame stability if someone wants to measure pollutant then global reaction parameter, Zeldovich reactor. And these are some of the applications.

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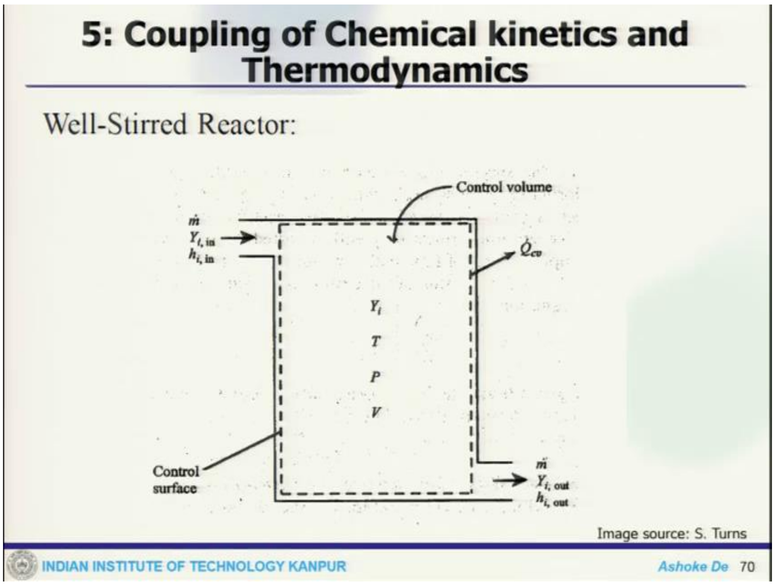

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Well-Stirred Reactor:

Image source: S. Turns

Now, this is the picture of the well stirred reactor with the electron species are coming in there is a going out this is a control volume. And the things are well mixed inside that.

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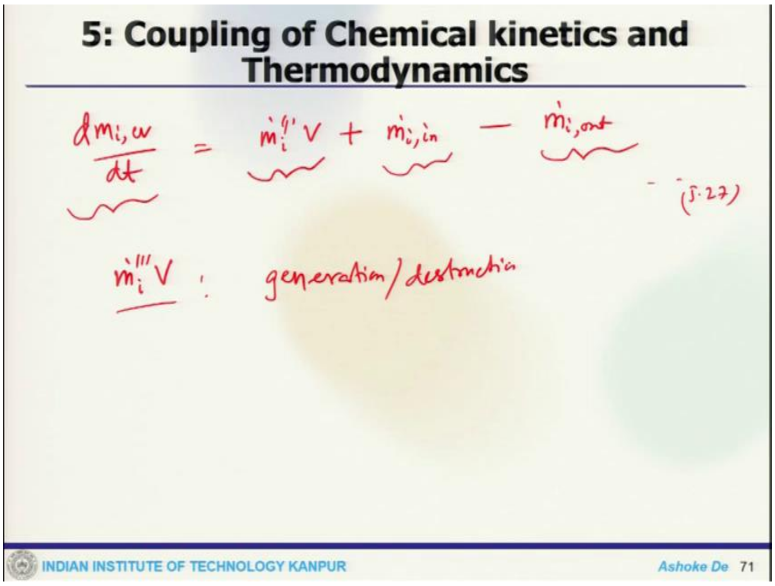

5: Coupling of Chemical kinetics and Thermodynamics

$$\underbrace{\frac{dm_{i,cv}}{dt}}=\underbrace{\dot m_i'''V}+\underbrace{\dot m_{i,in}}-\underbrace{\dot m_{i,out}} \quad - (5.27)$$

$\underline{\dot m_i'''V}$: generation/destruction

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So, again the mass conservation for any arbitrary species that one can write:

$$\frac{dm_{i,CV}}{dt}=\dot{m}_i'''V+\dot{m}_{i,in}-\dot{m}_{i,out}$$

So, this rate at which the mass of is generated this is mass of the flow of i which comes into the control volume. This is what goes out of the; and this is the rate at which this changes that you get the now $(\dot{m}_i'''V)$ this is the source term essentially this is either generation or destruction of species by chemical reaction through transformation of one species to another species.

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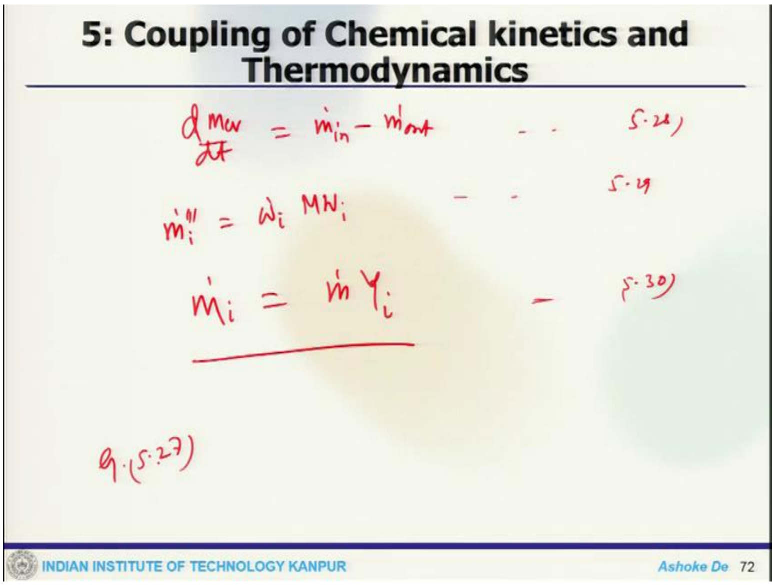

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$$\frac{dm_{cv}}{dt}=\dot m_{in}-\dot m_{out} \quad - - (5.28)$$

$$\dot m_i'''=\dot\omega_i MW_i \quad - - (5.29)$$

$$\underline{\dot m_i=\dot m Y_i} \quad - (5.30)$$

Eq.(5.27)

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Now also we can write that:

$$\frac{dm_{CV}}{dt} = \dot{m}_{i,in} - \dot{m}_{i,out}$$

And when you related this with the reaction rate so this is molecular weight and we can write that. And regarding the diffusion flux what can write that:

$$\dot{m}_{in} = \dot{m}Y_i$$

This is by ignoring the diffusion flux. Now, one can apply equation 5.27 to well stirred reactor and the time derivative on left hand side for steady state. This is one can use that, so with, now combining this equation, combining 5.29 5.30 and 5.27.

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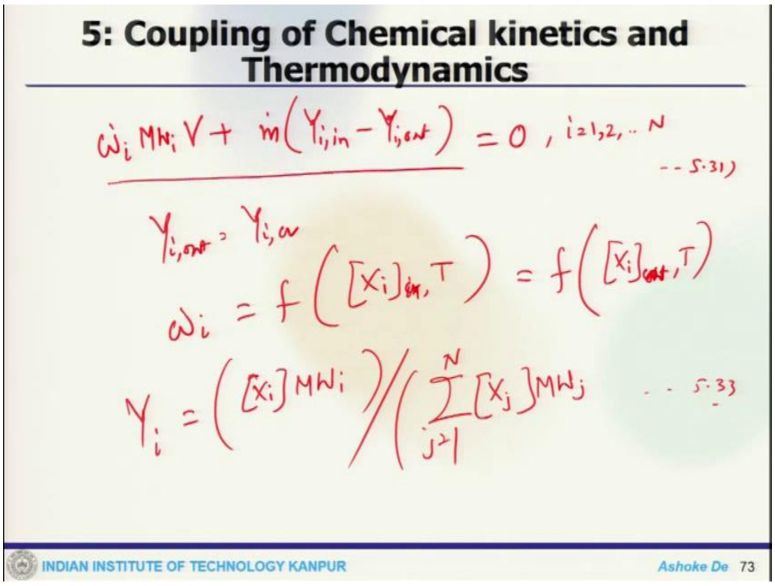

5: Coupling of Chemical kinetics and Thermodynamics

$$\dot{\omega}_i MW_i V + \dot{m}(Y_{i,in} - Y_{i,out}) = 0 \ , \ i=1,2,..N \quad --5.31)$$

$$Y_{i,out} = Y_{i,cv}$$

$$\dot{\omega}_i = f([X_i]_{cv}, T) = f([X_i]_{out}, T)$$

$$Y_i = ([X_i]MW_i) / \left(\sum_{j=1}^{N}[X_j]MW_j\right) \quad ..5.33$$

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So, one can write that:

$$\dot{\omega}_i MW_i V + \dot{m}(Y_{i,in} - Y_{i,out}) = 0$$

Where i is 1, 2 to N. So, further $Y_{i,out}$ is $Y_{i,in}$ of the control volume and species production rate:

$$\dot{\omega}_i = f([X_i]MW_i)$$

At the constant volume and temperature which is also a function of constant volume out and this is in that is out, where Y_i is:

$$Y_i = {([X_i]MW_i)}\Big/{\left(\sum_{j=1}^{N}[X_j]MW_j\right)}$$

So, this is what one can get it out now 5.31 here this can be written for N number of species provide N number of equation. This equation is valid for 1 to N and there would be N + 1 unknown, assuming $\dot{m}$ and V are known.

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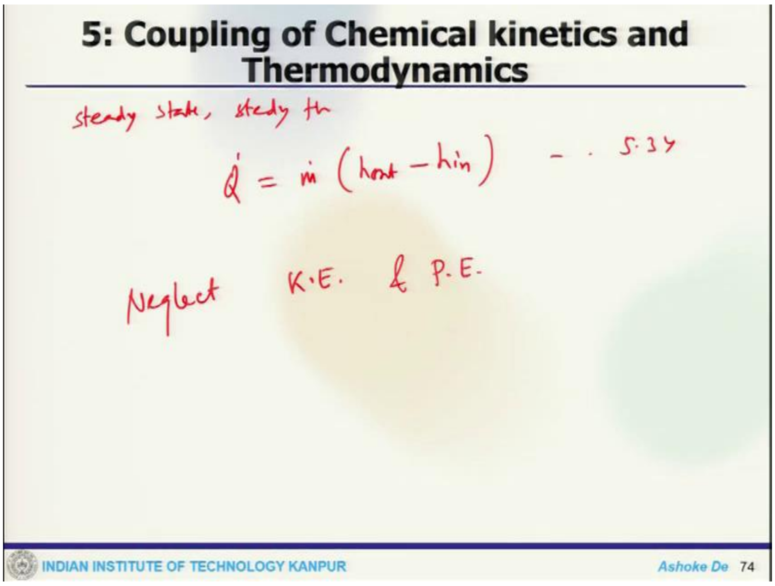

5: Coupling of Chemical kinetics and Thermodynamics

steady state, stedy flow

$$\dot{Q} = \dot{m}\left(h_{out} - h_{in}\right) \quad -- . \; 5.34$$

Neglect K.E. & P.E.

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So, the additional equation comes from the energy. Now what we can write that steady state steady flow energy conservation for well stirred reactor where we get:

$$\dot{Q} = \dot{m}(h_{out} - h_{in})$$

Which neglect any changes in kinetic and potential energy. Now in terms of individual species so this neglect kinetic energy and potential energy.

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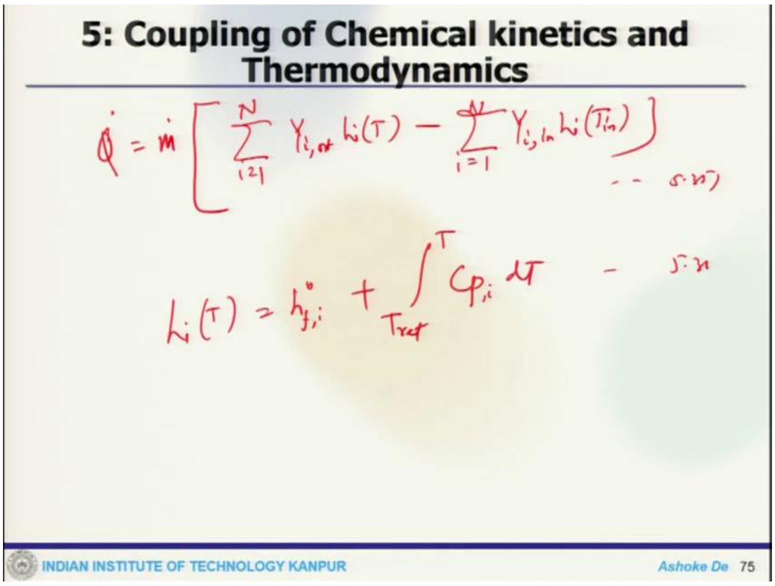

5: Coupling of Chemical kinetics and Thermodynamics

$$\dot{Q} = \dot{m}\left[\sum_{i=1}^{N} Y_{i,out} h_i(T) - \sum_{i=1}^{N} Y_{i,in} h_i(T_{in})\right] \quad -- \; 5.35$$

$$h_i(T) = h^{\circ}_{f,i} + \int_{T_{ref}}^{T} c_{p,i}\, dT \quad - \; 5.36$$

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So, now in terms of individual species, this equation 5.34 becomes:

$$\dot{Q} = \dot{m}\left[\sum_{i=1}^{N} Y_{i,out} h_i(T) - \sum_{i=1}^{N} Y_{i,in} h_i(T)\right]$$

So here, $h_i(T)$ is the sum of enthalpy of formation and $C_{pi}dT$. So, finding T and $Y_{i,out}$ is similar to equilibrium flame calculation but the composition is constant by kinetics.

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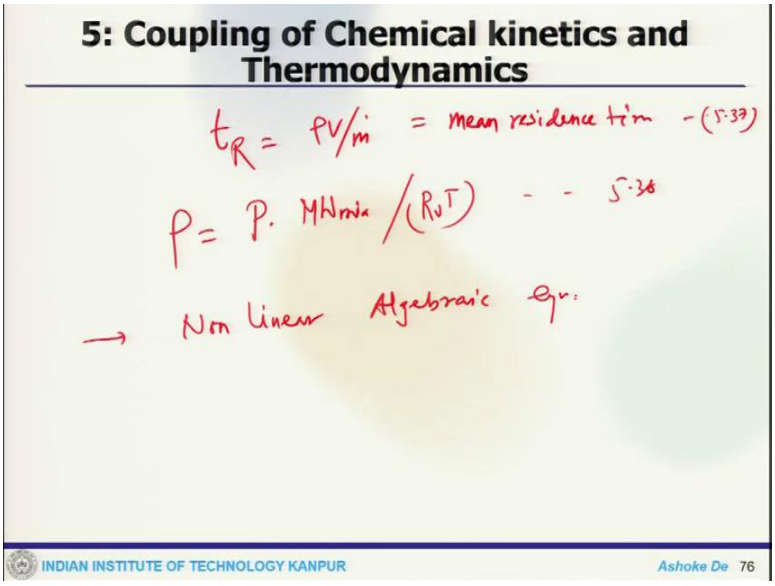

5: Coupling of Chemical kinetics and Thermodynamics

$t_R = \rho V/\dot{m}$ = mean residence tim - (5.37)

$\rho = P.\ MW_{mix}/(R_u T)$ - - 5.38

→ Non linear Algebraic eqn.

So most of the time in this mean residence is defined for well stirred reactor and that is:

$$t_R = {}^{\rho V}/_{\dot{m}}$$

So, this is mean residence time. Now at the mixture density is:

$$\rho = {}^{P.MW_{mix}}/_{(R_u T)}$$

For the well stirred reactor, equation system are nonlinear algebraic equations.

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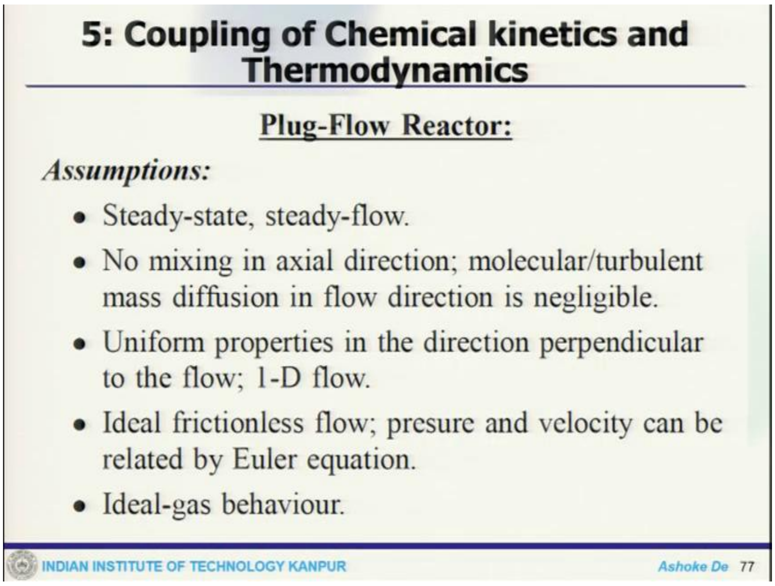

5: Coupling of Chemical kinetics and Thermodynamics

Plug-Flow Reactor:

Assumptions:

- Steady-state, steady-flow.
- No mixing in axial direction; molecular/turbulent mass diffusion in flow direction is negligible.
- Uniform properties in the direction perpendicular to the flow; 1-D flow.
- Ideal frictionless flow; presure and velocity can be related by Euler equation.
- Ideal-gas behaviour.

Now we will go to the plug flow reactor.

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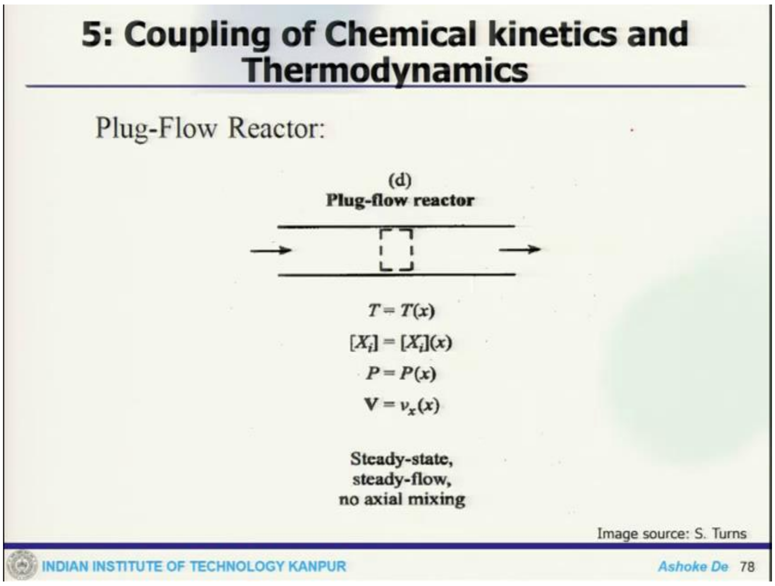

5: Coupling of Chemical kinetics and Thermodynamics

Plug-Flow Reactor:

$T = T(x)$

$[X_i] = [X_i](x)$

$P = P(x)$

$\mathbf{V} = v_x(x)$

Steady-state,
steady-flow,
no axial mixing

Image source: S. Turns

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So, the plug flow reactor is like that where is the mass coming in going out? They are the steady state flow but no axial mixing. So, the assumption are steady-flow, no mixing in the axial direction. Molecular and turbulent mass diffusion in flow direction is also negligible. Uniform properties in the direction perpendicular to the flow that means it essentially talks about one dimensional flow, ideal frictionless flow, pressure-velocity can be related by Euler equation and it follows ideal gas behaviour. So that is the schematic of the system.

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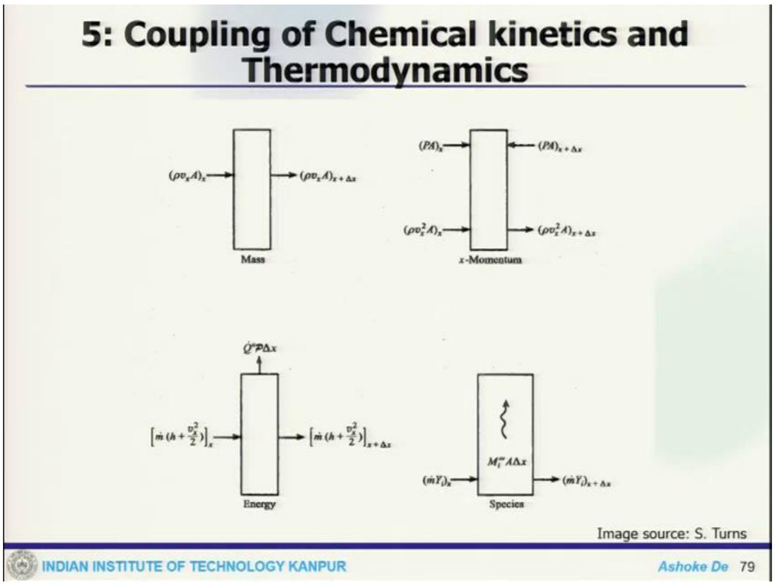

5: Coupling of Chemical kinetics and Thermodynamics

Image source: S. Turns

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Ashoke De 79

Basically write down for Mass conservation so that is the control volume issued whatever comes in it goes basically this is x and this is x + Δx. So that sleep is for small infinitesimal element of Δx with, it is mass conservation. And there will be momentum conservation and then there will be energy conservation this much of energy coming this is going out if there is a heat transfer takes place.

And finally species conservation comes and goes out and some generation or destruction. So, these are the four governing equations one requires. One is the mass, momentum, energy, species mass transfer equation.

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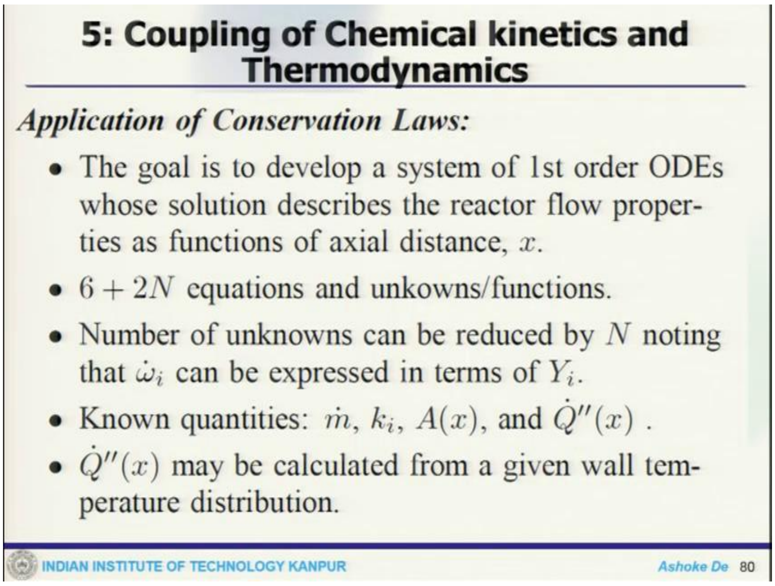

5: Coupling of Chemical kinetics and Thermodynamics

Application of Conservation Laws:

- The goal is to develop a system of 1st order ODEs whose solution describes the reactor flow properties as functions of axial distance, x.
- $6 + 2N$ equations and unkowns/functions.
- Number of unknowns can be reduced by N noting that $\dot{\omega}_i$ can be expressed in terms of Y_i.
- Known quantities: $\dot{m}$, k_i, $A(x)$, and $\dot{Q}''(x)$.
- $\dot{Q}''(x)$ may be calculated from a given wall temperature distribution.

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So what is the idea ideas to develop a system of first order ODE whose solution describe the reactor flow properties as a function of axial distance. Total we have 6 + 2 in equation and unknown of function show. The number of unknown can be reduced by N noting that $\dot{\omega}_i$ can be expressed in terms of Y_i and known quantities are $\dot{m}$, k_i, A(x) and $\dot{Q}''(x)$. So, this one can calculate from the given wall temperature distribution.

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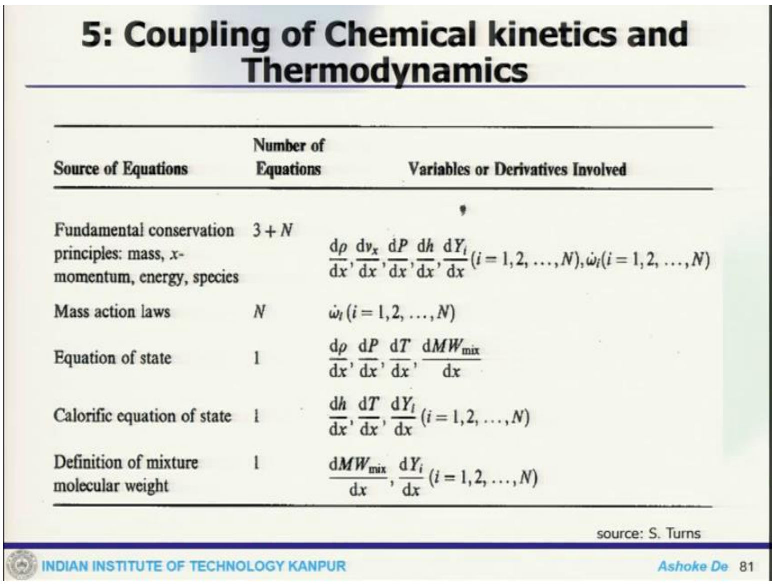

5: Coupling of Chemical kinetics and Thermodynamics

Source of Equations	Number of Equations	Variables or Derivatives Involved
Fundamental conservation principles: mass, x-momentum, energy, species	$3+N$	$\frac{d\rho}{dx}, \frac{dv_x}{dx}, \frac{dP}{dx}, \frac{dh}{dx}, \frac{dY_i}{dx}(i=1,2,\ldots,N), \dot{\omega}_i(i=1,2,\ldots,N)$
Mass action laws	N	$\dot{\omega}_i\,(i=1,2,\ldots,N)$
Equation of state	1	$\frac{d\rho}{dx}, \frac{dP}{dx}, \frac{dT}{dx}, \frac{dMW_{\text{mix}}}{dx}$
Calorific equation of state	1	$\frac{dh}{dx}, \frac{dT}{dx}, \frac{dY_i}{dx}\,(i=1,2,\ldots,N)$
Definition of mixture molecular weight	1	$\frac{dMW_{\text{mix}}}{dx}, \frac{dY_i}{dx}\,(i=1,2,\ldots,N)$

source: S. Turns

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Now these are the fundamental conservation mass, momentum, energy species. So, the number of equations are 3 + N under variables are derivative involve are $\frac{d\rho}{dx}, \frac{dP}{dx}, \frac{dh}{dx}$ and Y_i. This is for number of species and mass action law or mass conservation in which is $\dot{\omega}_i$ the variables equation of state one which contents is derivatives $\frac{d\rho}{dx}, \frac{dP}{dx}, \frac{dT}{dx}$ and this Calorific equation of state and the definition of mixture molecular weight.

So, these are only the source of equation number of equations and the variables which are involved.

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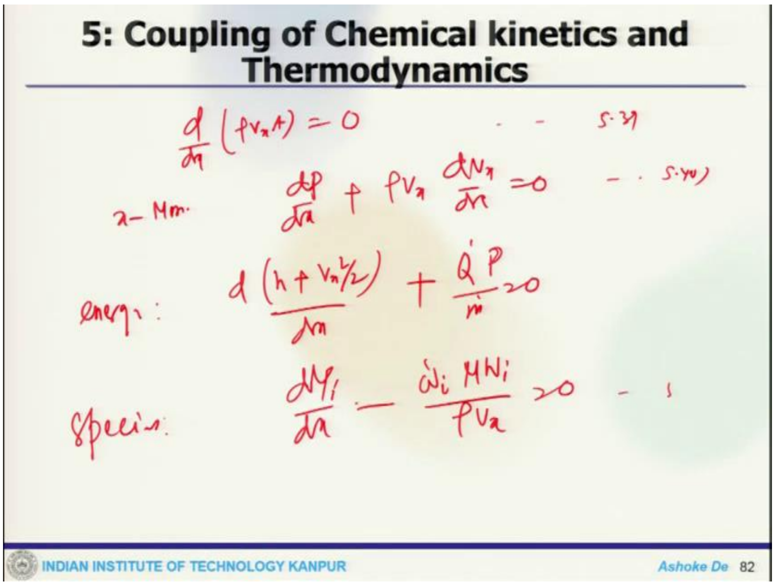

5: Coupling of Chemical kinetics and Thermodynamics

$$\frac{d}{dx}(\rho v_x A) = 0 \quad \text{- - } 5.37$$

x- Mm.

$$\frac{dP}{dx} + \rho v_x \frac{dv_x}{dx} = 0 \quad \text{- . } 5.40)$$

energy:

$$\frac{d\left(h + v_x^2/2\right)}{dx} + \frac{\dot{Q}' P}{\dot{m}} = 0$$

species:

$$\frac{dY_i}{dx} - \frac{\dot{\omega}_i MW_i}{\rho v_x} = 0 \quad \text{- } 1$$

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Now mass conservation you get:

$$\frac{d}{dx}(\rho V_x A) = 0$$

That is your 5.39 then X momentum equation you get:

$$\frac{dP}{dx} + \rho V_x \frac{dV_x}{dx} = 0$$

And then energy you get:

$$\frac{d\left(h + {V_x^2}/{2}\right)}{dx} + \frac{\dot{Q}P}{\dot{m}} = 0$$

So V_x is axial value and P is the local parameter. And species conservation:

$$\frac{dY_i}{dx} - \frac{\dot{\omega}_i MW_i}{\rho V_x} = 0$$

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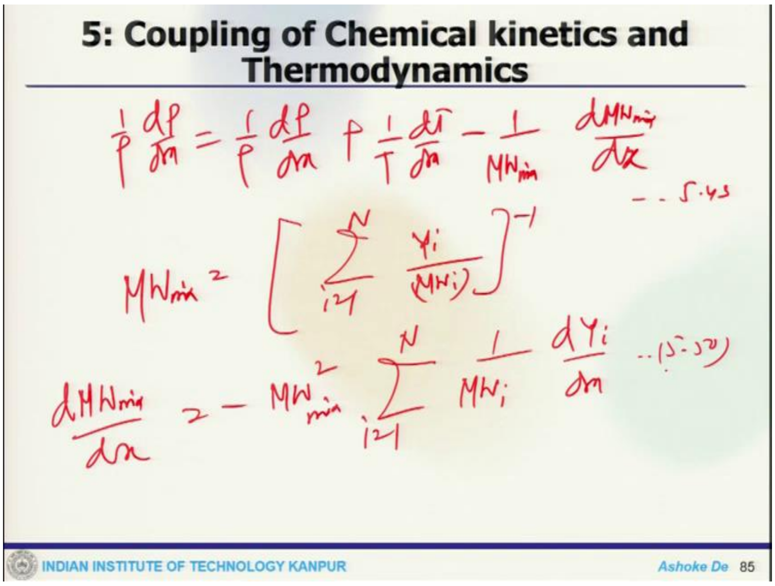

5: Coupling of Chemical kinetics and Thermodynamics

$$\frac{1}{\rho}\frac{d\rho}{dx} = \frac{1}{P}\frac{dP}{dx} + \frac{1}{T}\frac{dT}{dx} - \frac{1}{MW_{mix}}\frac{dMW_{mix}}{dx} \quad \text{-- 5.43}$$

$$MW_{mix} = \left[\sum_{i=1}^{N} \frac{Y_i}{(MW_i)}\right]^{-1}$$

$$\frac{dMW_{mix}}{dx} = -MW_{mix}^2 \sum_{i=1}^{N} \frac{1}{MW_i}\frac{dY_i}{dx} \quad \text{-- (5.50)}$$

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So, now equation 5.39 to 5.41one can rearrange and get that:

$$\frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{V_x}\frac{dV_x}{dx} + \frac{1}{A}\frac{dA}{dx} = 0$$

And one write:

$$\frac{dh}{dx} + V_x\frac{dV_x}{dx} + \frac{\dot{Q}''P}{\dot{m}} = 0$$

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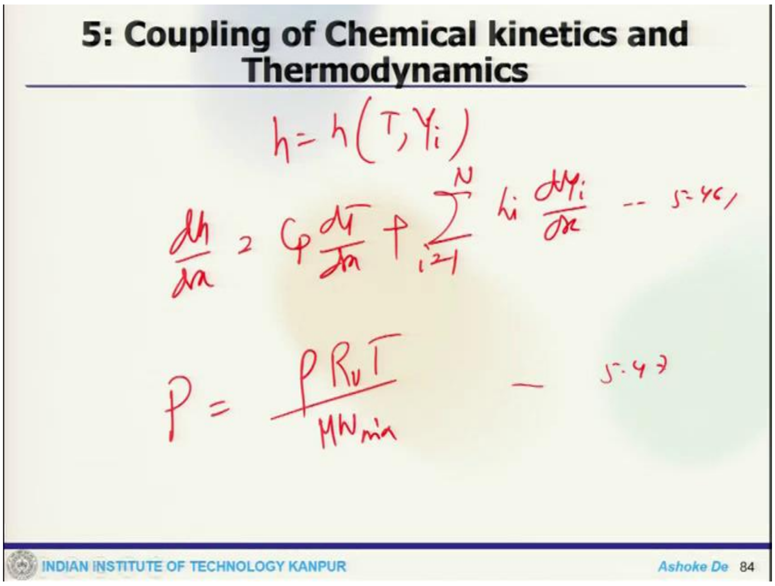

5: Coupling of Chemical kinetics and Thermodynamics

$$h = h(T, Y_i)$$

$$\frac{dh}{dx} = C_p \frac{dT}{dx} + \sum_{i=1}^{N} h_i \frac{dY_i}{dx} \quad \text{-- 5.46}$$

$$P = \frac{\rho R_u T}{MW_{mix}} \quad \text{— 5.47}$$

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So, using the ideal calorific equation where h is a function of temperature and the mass fraction. So, $\frac{dh}{dx}$ can be related as:

$$\frac{dh}{dx} = C_P \frac{dT}{dx} + \sum_{i=1}^{N} h_i \frac{dY_i}{dx}$$

So, to complete the mathematical description one more require is that for ideal gas law which is this.

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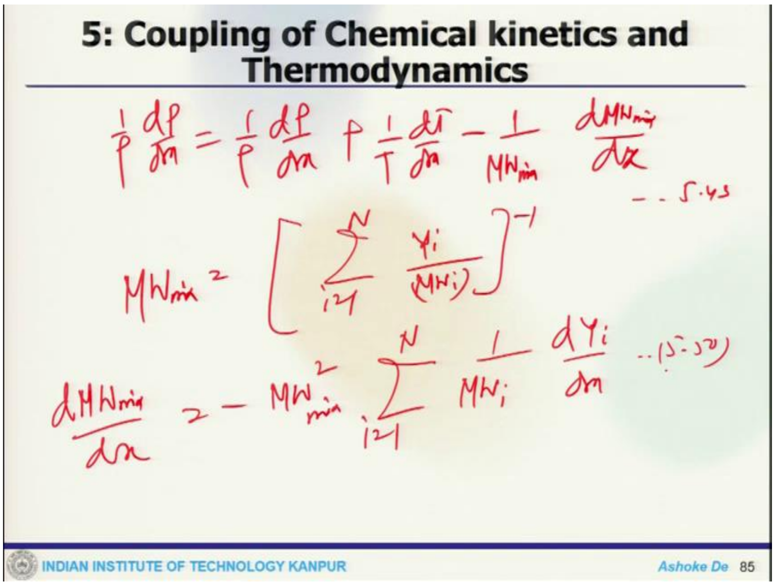

5: Coupling of Chemical kinetics and Thermodynamics

$$\frac{1}{P}\frac{dP}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx} - \frac{1}{MW_{mix}}\frac{dMW_{mix}}{dx} \quad \text{-- 5.48}$$

$$MW_{mix} = \left[\sum_{i=1}^{N} \frac{Y_i}{(MW_i)}\right]^{-1}$$

$$\frac{dMW_{mix}}{dx} = -MW_{mix}^2 \sum_{i=1}^{N} \frac{1}{MW_i}\frac{dY_i}{dx} \quad \text{..(5.50)}$$

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Ashoke De 85

So, these are the set of equation and so one will get:

$$\frac{1}{\rho}\frac{dP}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx} - \frac{1}{MW_{mix}}\frac{dMW_{mix}}{dx} = 0$$

Where

$$MW_{mix} = \left[\sum_{i=1}^{N} \frac{Y_i}{MW_i}\right]^{-1}$$

And these are:

$$\frac{dMW_{mix}}{dx} = -MW_{mix}^2 \sum_{i=1}^{N} \frac{1}{MW_i}\frac{dY_i}{dx}$$

Now number of equations which are here are basically can be reduced by eliminating some of the derivative by substitution.

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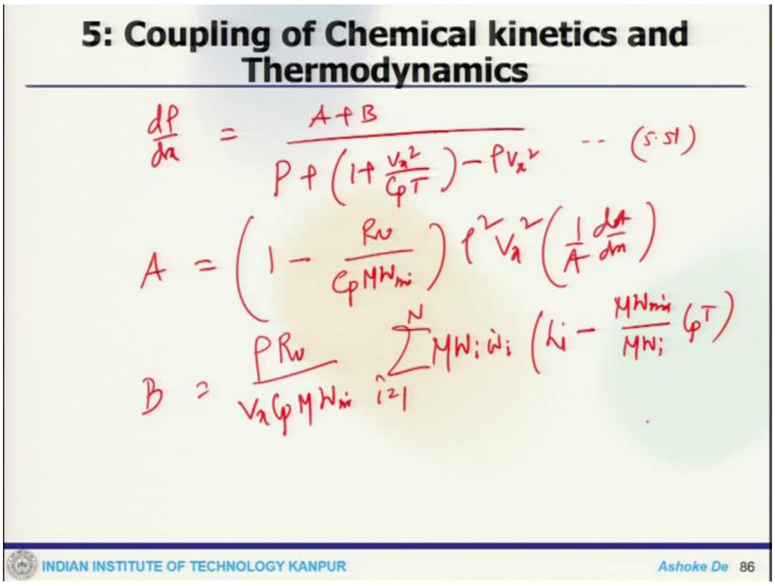

5: Coupling of Chemical kinetics and Thermodynamics

$$\frac{d\rho}{dx} = \frac{A+B}{P + \left(1+\frac{V_x^2}{C_pT}\right) - \rho V_x^2} \quad \text{-- (5.51)}$$

$$A = \left(1 - \frac{R_u}{C_p MW_{mix}}\right)\rho^2 V_x^2 \left(\frac{1}{A}\frac{dA}{dx}\right)$$

$$B = \frac{\rho R_u}{V_x C_p MW_{mix}} \sum_{i=1}^{N} MW_i \omega_i \left(h_i - \frac{MW_{mix}}{MW_i} C_p T\right)$$

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And one can find out:

$$\frac{d\rho}{dx} = \frac{A + B}{P + \left(1 + \frac{V_x^2}{C_P T}\right) - \rho V_x^2}$$

So, this is what you get where A is:

$$A = \left(1 - \frac{R_u}{C_p MW_{mix}}\right)\rho^2 V_x^2 \left(\frac{1}{A}\frac{dA}{dx}\right)$$

And

$$B = \frac{\rho R_u}{V_x C_p MW_{mix}} \sum_{i=1}^{N} MW_i \dot{\omega}_i \left(h_i - \frac{MW_{mix}}{MW_i} C_p T\right)$$

So, this is what you get and I will stop here and finish the rest of the derivation in the following lecture, thank you.