Turbulent Combustion: Theory and Modeling
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Lecture-15
Coupling of Chemical Kinetics and Thermodynamics (contd.) and Laminar Premixed Flames

Welcome back let us continues the discussion on coupling of chemical kinetics and the thermodynamics. So, we were in the middle of doing the discussion, we were looking some basic reactors and then doing the analysis. So, based on their assumption and other characteristics, so, the last one where we stopped while doing the plug flow reactor.

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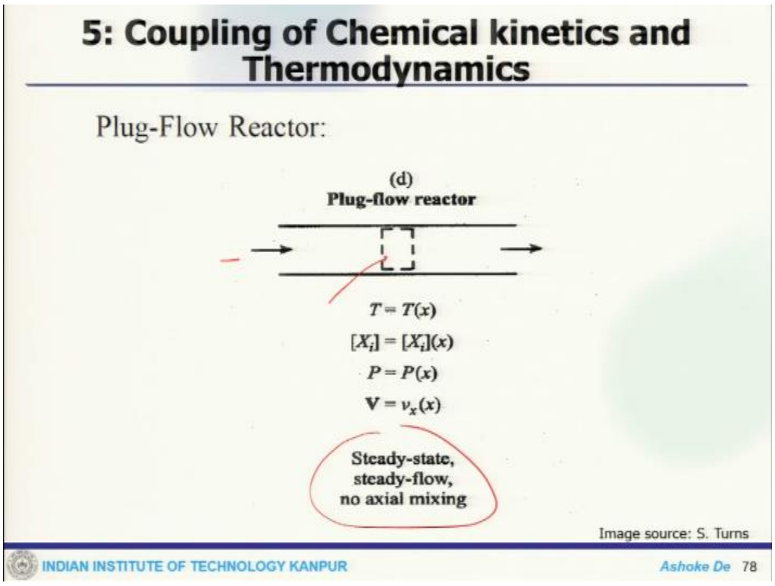
5: Coupling of Chemical kinetics and Thermodynamics

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

So, this is where we started off, this is the schematic of the plug flow reactor, where the species comes in and then goes out this is the control volume, small control volume and then there are some assumption which it is build upon steady state, steady flow, no axial mixing and all these.

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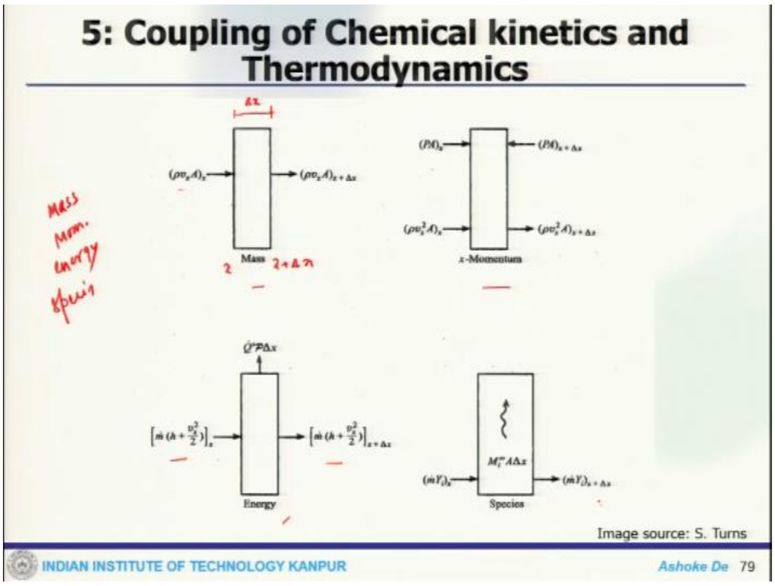

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Image source: S. Turns

Then what we are doing, there are basic conservation equation of mass conservation. So, this is the small element that we have taken and mass conservation, then momentum conservation and momentum only we are looking at the x momentum and then energy also where this is the energy flux comes in that goes out and the species mass transfer.

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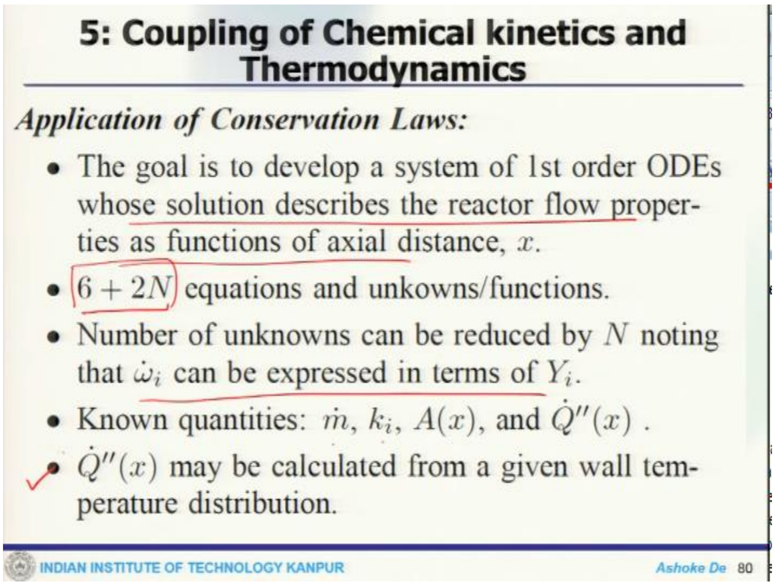

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Application of Conservation Laws:

- The goal is to develop a system of 1st order ODEs whose solution describes the reactor flow properties as functions of axial distance, x.
- $\boxed{6+2N}$ 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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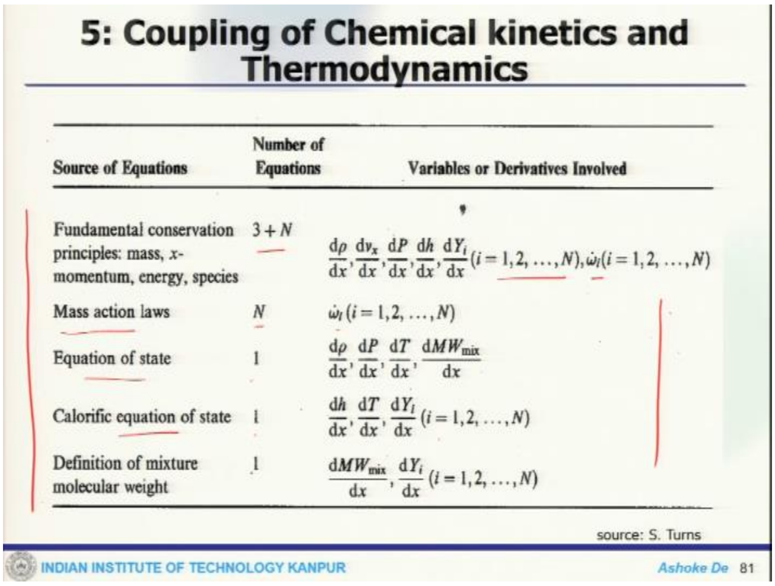

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Source of Equations	Number of Equations	Variables or Derivatives Involved
Fundamental conservation principles: mass, x-momentum, energy, species	$3+N$	$\frac{d\rho}{dx}, \frac{dv_x}{dx}, \frac{dP}{dx}, \frac{dh}{dx}, \frac{dY_i}{dx} (i=1,2,\ldots,N),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

source: S. Turns

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So, this we can look at the system with all that. So, this is the picture if you recall that these are the fundamental equations, where x momentum energy species, how many number of equations mass as N, equation of state, 1 calorific equation.

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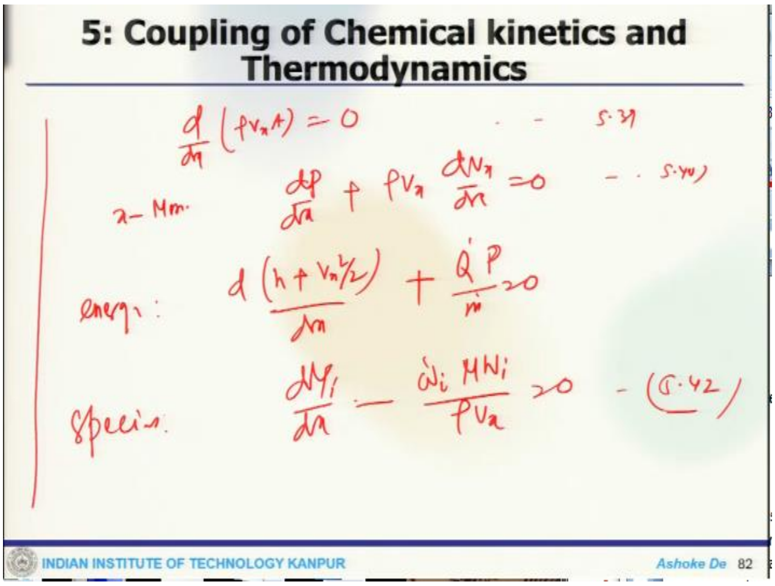

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$$\frac{d}{dx}(\rho v_x A) = 0 \quad \text{- - 5.39}$$

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: $$\frac{dY_i}{dx} - \frac{\dot{\omega}_i MW_i}{\rho v_x} = 0 \quad \text{- (5.42)}$$

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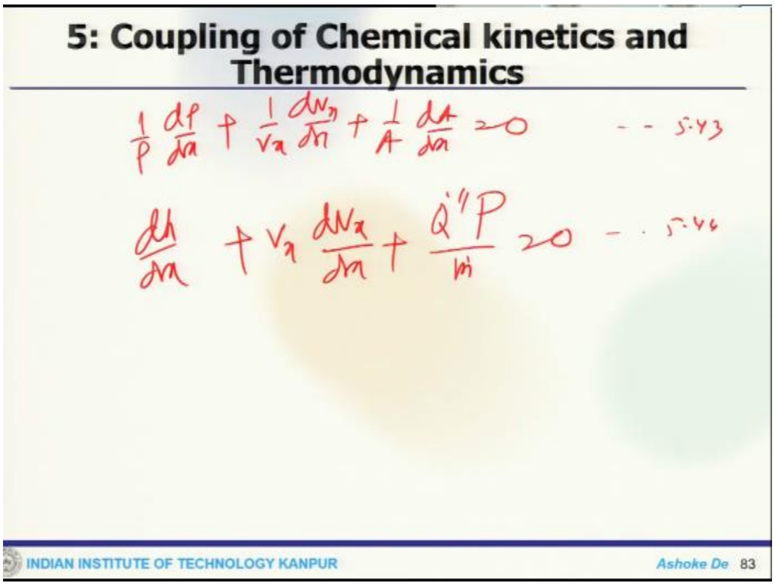

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$$\frac{1}{P}\frac{dP}{dx} + \frac{1}{V_x}\frac{dV_x}{dx} + \frac{1}{A}\frac{dA}{dx} = 0 \quad \text{-- 5.43}$$

$$\frac{dh}{dx} + V_x\frac{dV_x}{dx} + \frac{\dot{Q}''P}{\dot{m}} = 0 \quad \text{-- 5.46}$$

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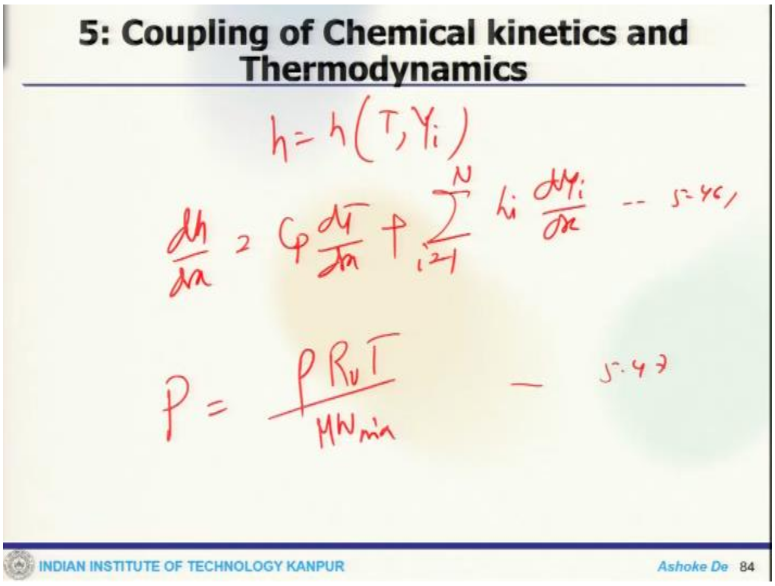

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$$h = h(T, Y_i)$$

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

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

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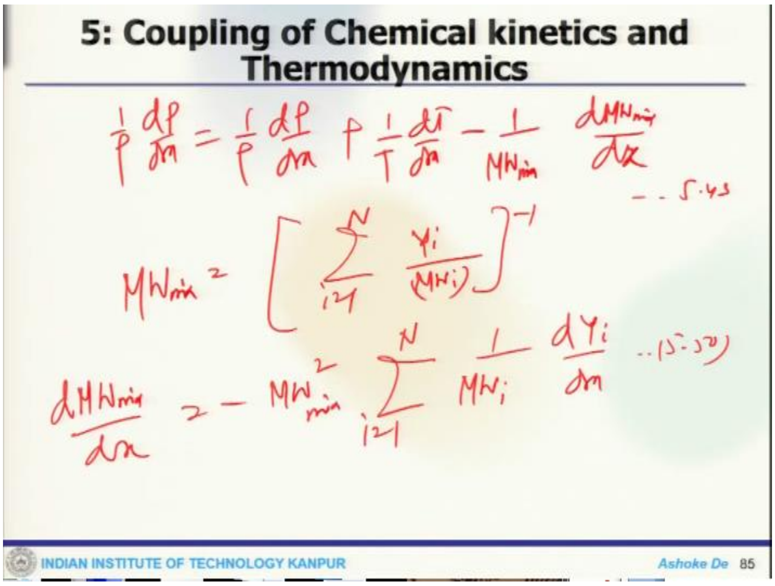

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$$\frac{1}{\rho}\frac{d\rho}{dx} = \frac{1}{P}\frac{dP}{dx} + \frac{1}{T}\frac{dT}{dx} - \frac{1}{MW_{mix}}\frac{dMW_{mix}}{dx} \quad \text{-- 5.45}$$

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

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

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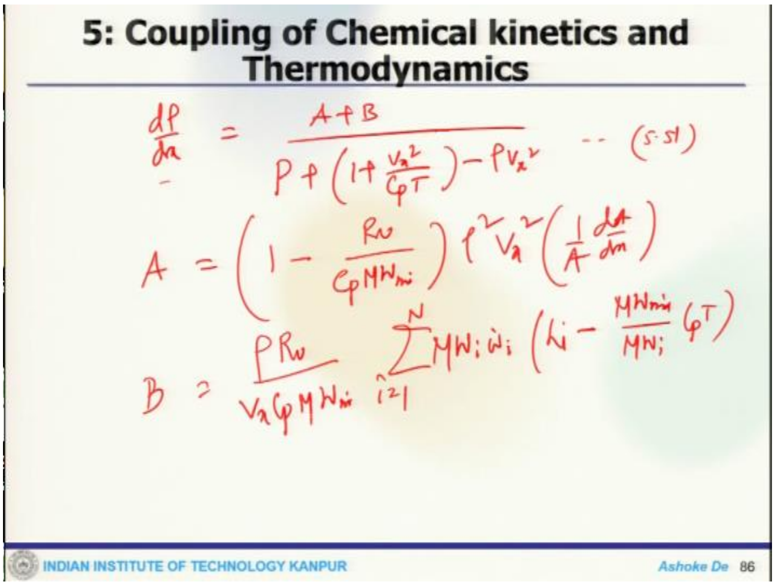

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$$\frac{dP}{dx} = \frac{A+B}{P + \left(1+\frac{V_x^2}{C_pT}\right) - \rho V_x^2} \quad \text{-- } (5.51)$$

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

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

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So, using this concept, we started the set of equation and then finally, we derived and we stopped here, where you get $\frac{dP}{dx}$ in terms of some coefficients A and B and obviously, the other parameters like actual velocity, thermodynamic parameter, temperature, C_p and all these are there were A is like this and B is integrant like this,

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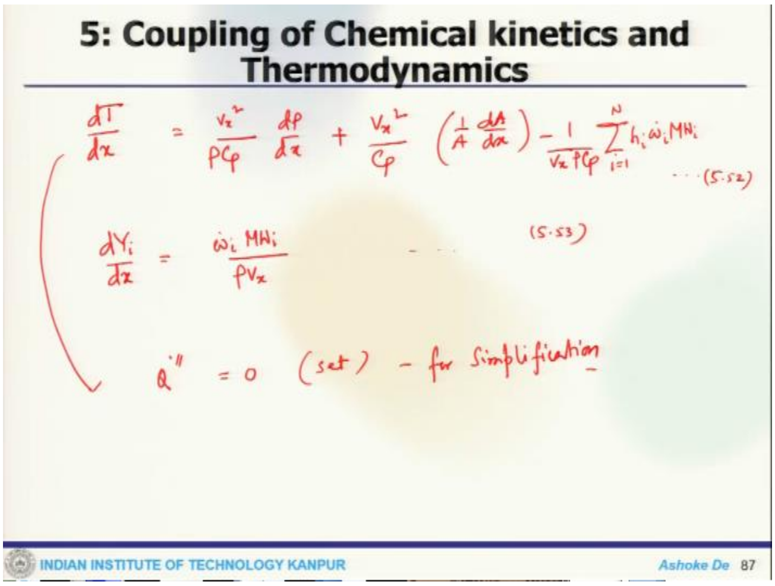

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$$\frac{dT}{dx} = \frac{V_x^2}{\rho C_p}\frac{dP}{dx} + \frac{V_x^2}{C_p}\left(\frac{1}{A}\frac{dA}{dx}\right) - \frac{1}{V_x \rho C_p}\sum_{i=1}^{N} h_i \dot{\omega}_i MW_i \quad \cdots (5.52)$$

$$\frac{dY_i}{dx} = \frac{\dot{\omega}_i MW_i}{\rho V_x} \quad \cdots (5.53)$$

$\dot{Q}'' = 0$ (set) - for simplification

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Now, we can look at the temperature gradient. So, that would look like now:

$$\frac{dT}{dx} = \frac{V_x^2}{\rho C_P}\frac{dP}{dx} + \frac{V_x^2}{C_P}\left(\frac{1}{A}\frac{dA}{dx}\right) - \frac{1}{V_x \rho C_P}\sum_{i=1}^{N} h_i \dot{\omega}_i MW_i$$

So this your equation number 52 and the species conservation equation will comes down to:

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

This would be your equation number 53. So, what you can note here in this particular equation, so, there $\dot{Q}''$ has been set to 0, this is for simplification. So, now one can calculate the residence time.

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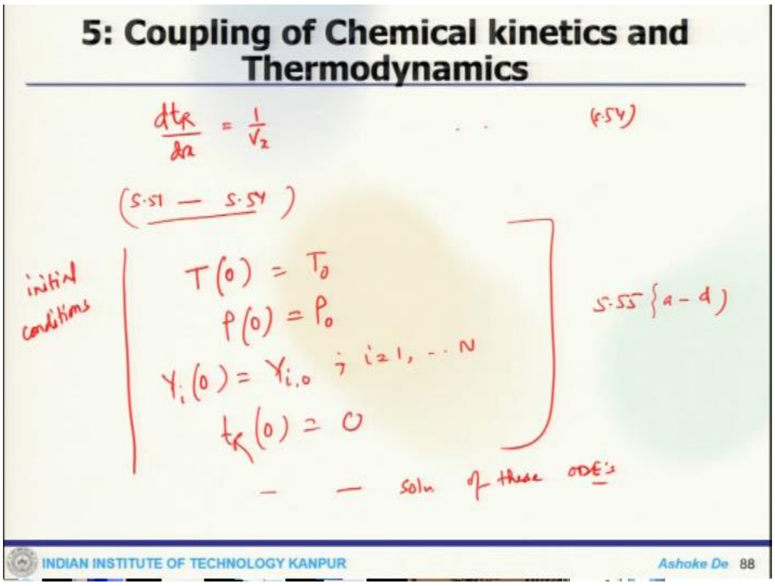

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$$\frac{dt_R}{dx} = \frac{1}{V_x} \quad \cdots (5.54)$$

(5.51 — 5.54)

initial conditions

$$\left.\begin{aligned} T(0) &= T_0 \\ P(0) &= P_0 \\ Y_i(0) &= Y_{i,0} \; ; \; i = 1, \ldots N \\ t_R(0) &= 0 \end{aligned}\right] \quad 5.55\{a-d)$$

— — soln of these ODE's

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So, which adds one more equation, when you look at the residence time, this should be:

$$\frac{dt_R}{dx} = \frac{1}{V_x}$$

So, that is the residence time. Now, there are initial conditions. So, the equations 5.51 to 5.54 there are initial conditions which are essentially required to solve this equation, this is T_0 density will be ρ_0 Y_i is $Y_{i,0}$ for i is equal to 1 to N and t_R is 0.

So, this is your sets of equation from a to d. So, these are the initial conditions which talk about equation they are expose to and whether those equations can be solved based on these initial conditions. Now, once you have the initial condition, you can easily find out the solution of this ODE's because these are simple ODE's. So, using this one can find out the solution all these ODE's that will get you the temperature profile, a species profile and other things

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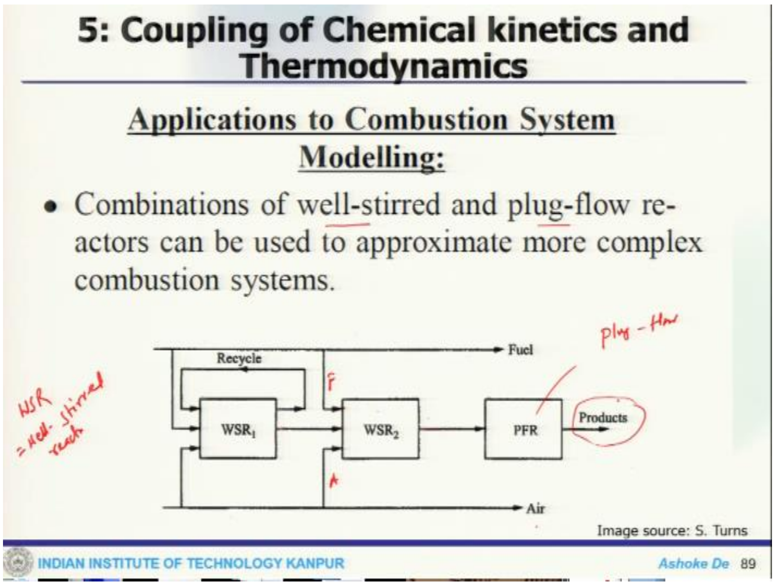

5: Coupling of Chemical kinetics and Thermodynamics

Applications to Combustion System Modelling:

- Combinations of well-stirred and plug-flow reactors can be used to approximate more complex combustion systems.

Image source: S. Turns

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Now, we can look at some of these applications to the combustion system modeling where we actually apply these things, because, what we looked at is the basic fundamental reactors like plug flow reactor, perfectly stirred reactor, constant volume reactor, constant pressure reactor. So, where do we use all these? So now, the combination of well-stirred reactor and plug flow reactors can be used to approximate more complex combustion system. For example, you have a fuel and this is here.

Now, this is one of the well stirred reactor. WSR stands for well stirred reactor, so this is the first WSR then there is a recycling or fuel comes in here, comes in some combustion product comes out, it gets into second well stirred reactor where again some amount of fuel and some amount of your goes in along with this combustion product. So, that means there are 3 limit again some amount of fresh fuel is coming in some amount of fresh air is coming in and the combustion product.

Then finally, this combustion product goes to plug flow reactor. So, this is plug flow reactors and then finally, you get the final set of products

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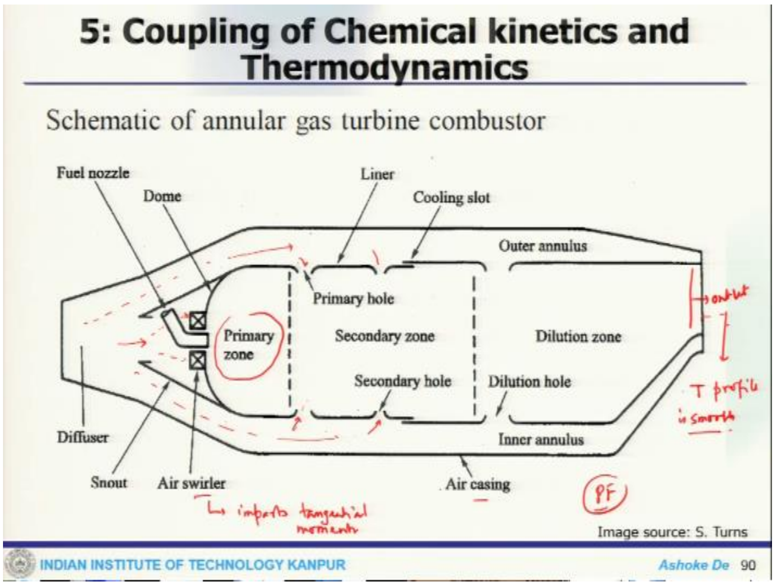

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Schematic of annular gas turbine combustor

Image source: S. Turns

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Now, look at slightly complicated example of gas turbine where you have so many different regime of thing. So, this is a schematic or the cut section of gas turbine combustor. So, if you look at this is the outer casing or other air casing first, portion here is the diffuser. So, in the diffuser, actually, if you look at realistically well flying, then you can see there is a fan also there which casing layer to the system then you have a fuel nozzle and some other covered snout and the swirler. So, the air comes in here that is allowed to pass to this swirler. So, when that pass through the swirler what it does, it actually imparts tangential momentum to the air and also so, essentially when you put so many in the energy to it, so, there will be pure 3 dimensional is this does a lot of things, I mean it not only allows to have rapid quick mixing also make the system more turbulent in nature.

So, there is a very specific purpose of using this kind of swirler and then the fuel comes in to that gets well mixed if it is a liquid fuel then that will atomize and evaporate and then the air is there. So, the primary zone there would be primary reaction going on. So, this is called the primary zone then these are the primary holes where again the air pass through and they are the liner and these are the secondary hole for the secondary hole allow some more air to come in because some air which is bypass there that goes to this casing and they goes to this holes. Now secondary air when it comes through they also take part in the secondary combustion or in the secondary zone combustion. So, whatever comes out from this side, this will also react with the excess air which is there are 2 purposes of say injecting the secondary injection or rather having the secondary injection. It will not only allow to have some reaction to take place, if there is some excess fuel. So, that would be burnt here because now you inject some more air to it.

Secondly, it will also mix with the hot product and little bit smooth out the temperature profile. So, that when it goes out and that is also done through other dilution hole also. So, at the end of this at the outlet, the idea is that wants needs to be they expectation is that the temperatures profile here at the outlet, that T profile should be smooth enough. So, that is the whole idea and to get that we do lot of dilution primary secondary injections. So, that I mean also there are other advantages of doing these multiple injections to these things. But at end of the day, what one have it a smoother T profile. So, once you have a smoother T profile, this will reduces your pattern factors and that is one of the biggest design fact concern for gas turbine. So, that is because this temperature outlet of the combustion product that actually goes to turbine. So we have already discussed turbine is the in a gas turbine plays a critical role because that dictates the stop the design issues.

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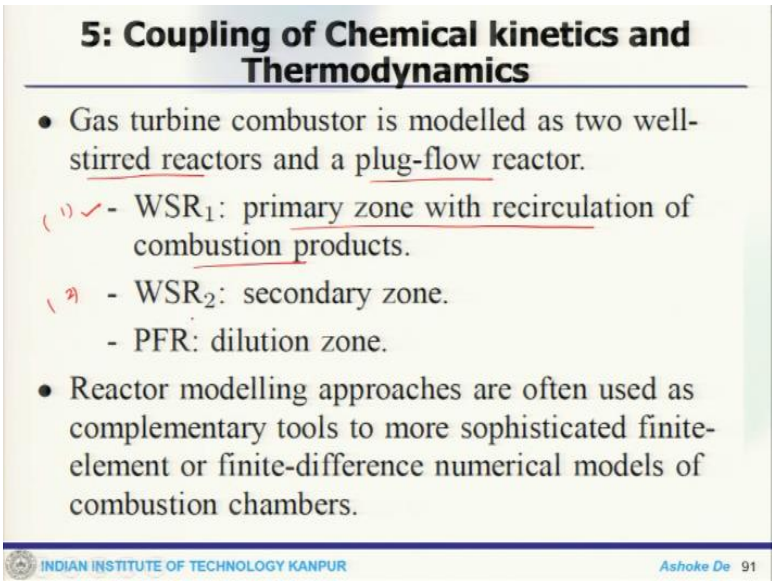

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- Gas turbine combustor is modelled as two well-stirred reactors and a plug-flow reactor.
  - (1) ✓ - WSR$_1$: primary zone with recirculation of combustion products.
  - (2) - WSR$_2$: secondary zone.
  - PFR: dilution zone.
- Reactor modelling approaches are often used as complementary tools to more sophisticated finite-element or finite-difference numerical models of combustion chambers.

Now, how we model these things, it is modeled as two well stirred reactor and a plug flow reactor. So, where are the well stirred reactor the primary zone is one of the well stirred reactors. So, primary zone with recirculation of the combustion product this is one well stirred reactor and the second well stirred reactor would be sitting in that. So, if you go back to the schematic

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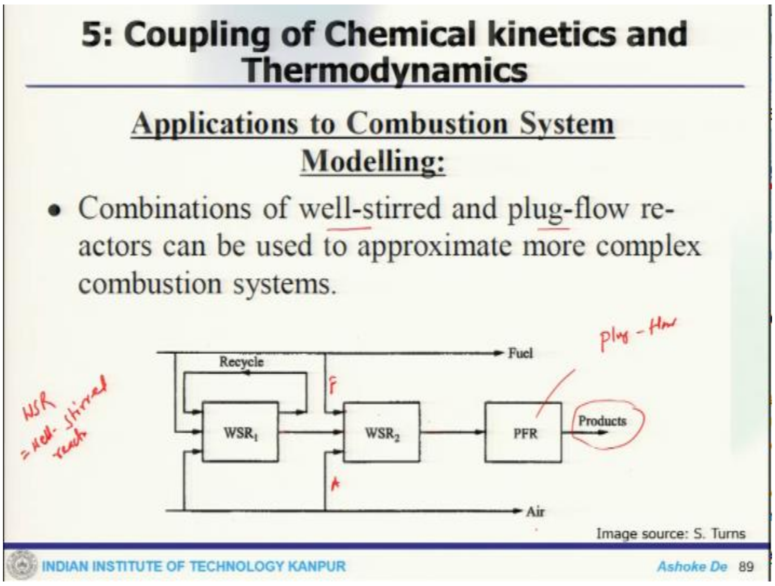

5: Coupling of Chemical kinetics and Thermodynamics

Applications to Combustion System Modelling:

- Combinations of well-stirred and plug-flow reactors can be used to approximate more complex combustion systems.

Image source: S. Turns

This is where air comes in fuel comes in. So, they react. The recycling is essentially nothing but that because of the swirling flow in circulation bubbles things being back. So, this is one well stirred reactor then you add some more fuel and this is second well stirred reactor and finally the plug flow reactor in the dilution engine. So, this reactor modeling uploads are often used as complimentary to the tools for more sophisticated final implement are different numerical models for combustion chamber.

So these are some things that one used to simplify a complicated problem like an gas turbine combustor. So, that is actually gives you an idea, this application of these basic or fundamental reactors, for the modeling purposes of the complicated system. So, though it is simplify system that can give you a fair amount of idea what goes on in the system, so that pretty much actually we want to talk about the coupling thing.

And then we will move to the next set of discussion, which will essentially because now we have finished all these basics of the combustion and all these things, basic thermodynamics basic properties, and now we will go to a very specific thing to explain.

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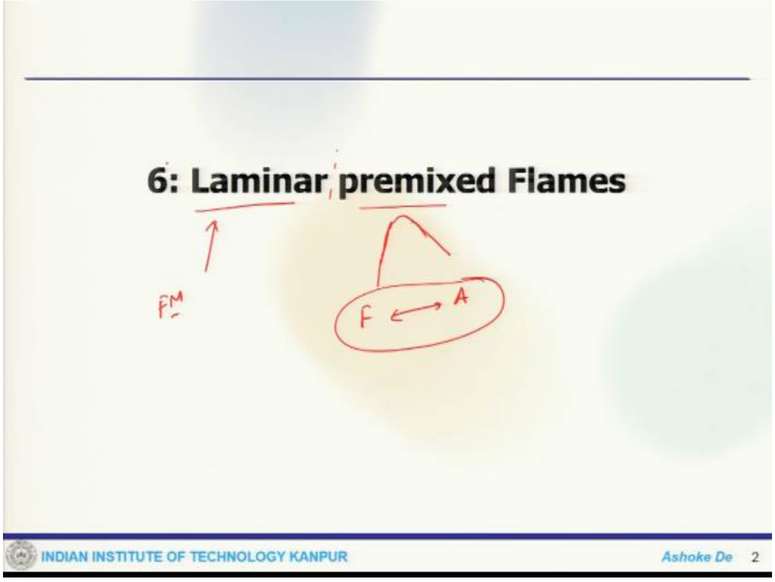

6: Laminar premixed Flames

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So laminar premixed flames. So, that means these talks about 2 things, one is the pre mixed that means my fuel in air. So, this gives me an idea that fuel and air there already mixed. So, that means they are mixed a priori and then send to the reacting zone or combustion zone or combustor laminar stands for because this is from your fuel mechanics. So, the fuel is laminar. So, essentially this immediately tells you as soon as you say laminar premixed that means that you can get some idea about the scales and all those things.

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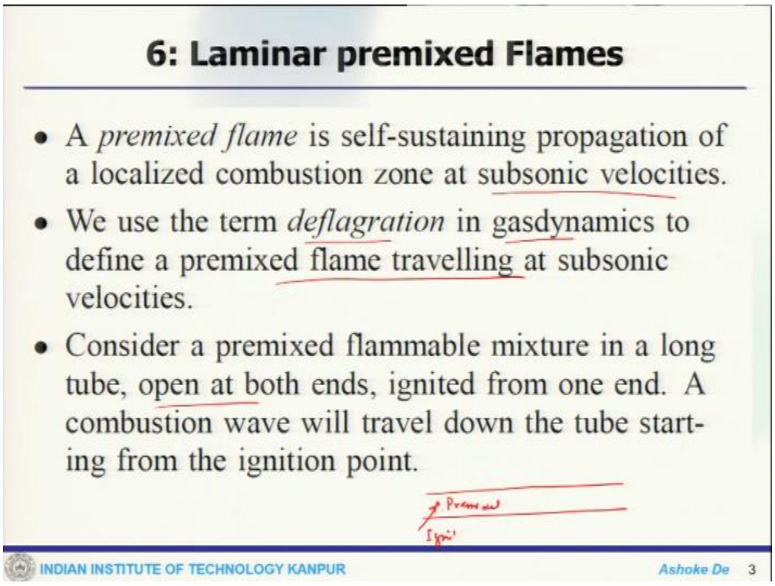

6: Laminar premixed Flames

- A *premixed flame* is self-sustaining propagation of a localized combustion zone at subsonic velocities.
- We use the term *deflagration* in gasdynamics to define a premixed flame travelling at subsonic velocities.
- Consider a premixed flammable mixture in a long tube, open at both ends, ignited from one end. A combustion wave will travel down the tube starting from the ignition point.

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So, let us go into that discussion. Now, there are certain important properties that one has to know before getting into the details of this premixed flame. So, one is that the premixed flame is self sustaining propagation of a localized combustion zone at subsonic velocities. So, this is an important point. So, that actually now we call it sometimes the deflagration in gas dynamics or compressible gas dynamics or to define a premixed flame travelling at subsonic speed.

Now, if you consider a premixed flammable mixture, in a long tube, open at both ends, that means, we are talking about the kind of a tube which is open at both ends, and you have a premixed mixture here and you ignite from one end then the combustion wave which will be generated due to this reaction that will travel down to the tube towards the other end from the starting point.

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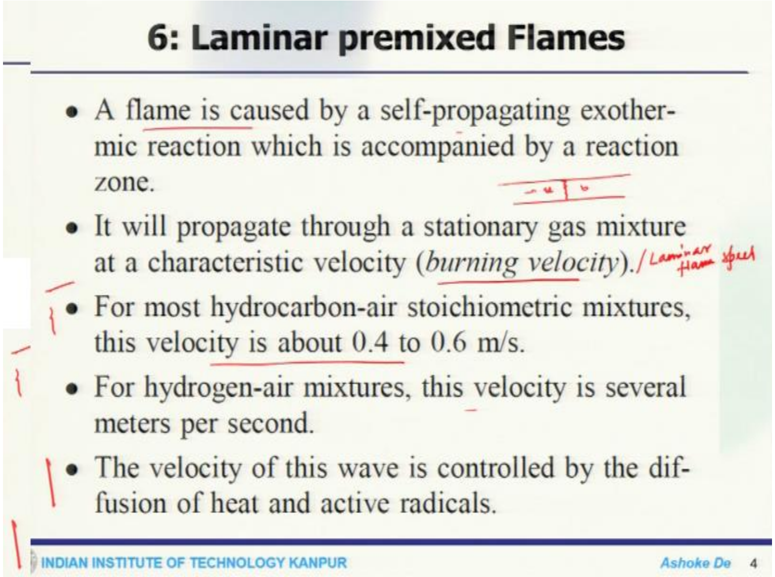

6: Laminar premixed Flames

- A flame is caused by a self-propagating exothermic reaction which is accompanied by a reaction zone.
- It will propagate through a stationary gas mixture at a characteristic velocity (*burning velocity*)./ Laminar flame speed
- For most hydrocarbon-air stoichiometric mixtures, this velocity is about 0.4 to 0.6 m/s.
- For hydrogen-air mixtures, this velocity is several meters per second.
- The velocity of this wave is controlled by the diffusion of heat and active radicals.

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Now, more to heat the flame is caused by a self propagating exothermic - reaction which is accompanied by a reaction zone that means, when this premixed mixture is ignited, the combustion wave in travel towards the other side then obviously, it will create some sort of an so, if you to passing through these tube somewhere it will create a thin reaction zone. So, one side of that would be burnt side other side would be unburnt side that means mixture comes in. So, it says self-sustaining or self-propagating system.

Now, it will propagate through stationary gas mixture at the characteristics velocity which is called burning velocity or laminar flame speed. So, this is one of the very fundamental property of a premixed flame and that one has to know now. Most hydrocarbon stoichiometric mixtures by velocity above this. So, that we will see how this burning velocity actually varies with a mixture or rather the stoichiometric mixture cohesion.

Now, when you talk about these are some essentially the comments and when talk above that hydrogen air mixtures compared to a hydrocarbon, fuel is burning velocities quite higher. And that happens because, once we will do that detailed analysis of this burning velocity will see that depends on the molecular weight, along with the mass diffusivity and hydrogen has much higher mass diffusivity.

Now, the velocity of this wave is also controlled by the diffusion of heat and active radicals that is always obvious, because once the reaction starts in any reacting system, there would be formation of radicals and active radicals and that will also produce some heat.

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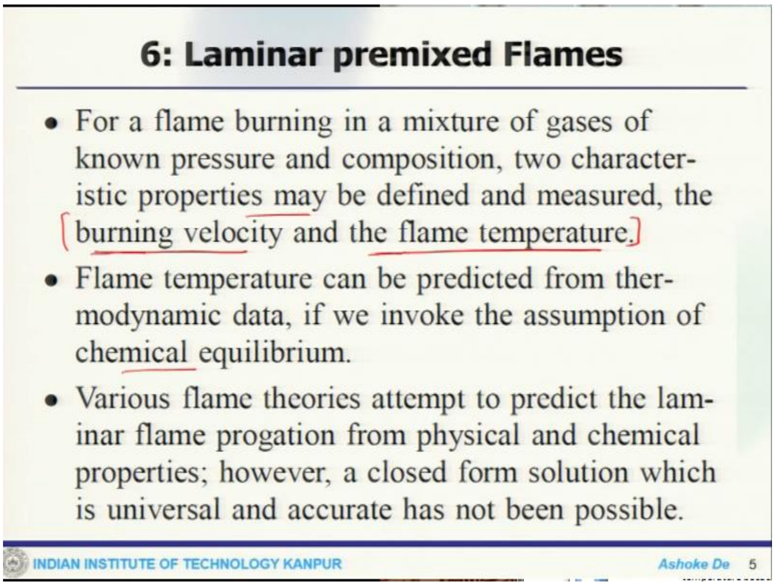

6: Laminar premixed Flames

- For a flame burning in a mixture of gases of known pressure and composition, two characteristic properties may be defined and measured, the burning velocity and the flame temperature.
- Flame temperature can be predicted from thermodynamic data, if we invoke the assumption of chemical equilibrium.
- Various flame theories attempt to predict the laminar flame progation from physical and chemical properties; however, a closed form solution which is universal and accurate has not been possible.

Now, when the flame is burning in a mixture of gases then the pressure and composition to characteristic properties can be defined and measured one is the burning velocity or flames speed or laminar flame speed, second is the flame temperature. So, now, that is always obvious. Now, when there is a reaction going on, obviously will have a temperature because these are mostly exothermic reaction and any exothermic reaction there will be heat release. So, when there is a heat release would be able to get some temperature.

So, that one may think about there is what is something very fancy about it. I mean, we will see, when you talk about the premixed mixture, it is slightly different and that is why flame temperature is allows obvious, but the important thing is the burning velocity and also flame thickness which will come to that. So, the temperature you can predict from the thermodynamic data and if you invoke also chemical equilibrium concept, you can do that.

But secondly, the prediction of the burning velocity people have predicted that thing through a lot of experimental observation, there are theoretical models and so, a lot of things which are present there for prediction of the burning velocity.

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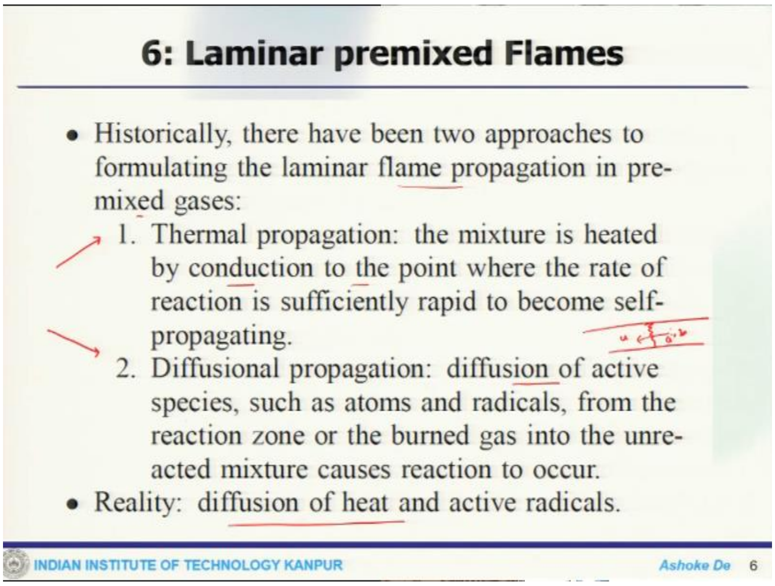

6: Laminar premixed Flames

- Historically, there have been two approaches to formulating the laminar flame propagation in premixed gases:
    1. Thermal propagation: the mixture is heated by conduction to the point where the rate of reaction is sufficiently rapid to become self-propagating.
    2. Diffusional propagation: diffusion of active species, such as atoms and radicals, from the reaction zone or the burned gas into the unreacted mixture causes reaction to occur.
- Reality: diffusion of heat and active radicals.

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Now, to go back a little bit to the history, there are essentially 2 approaches formulating the laminar flame propagation in premixed gases. First one, there is a hypothesis on which talks about thermal propagation that means, the mixture is heated by conduction to the point where the rate of reaction is sufficiently rapid to become self-propagating. So, that is a concept completely based on thermo analogy.

And the second one based on the diffusion of propagation, which talks about that diffusion of active species such as atoms and radicals from the reaction zone of the burnt gas into the unreacted mixture causes reaction to occur. So, there are 2 different thought process completely one is purely based on the thermal hypothesis, if you look at the system like this and this is the reaction zone this is unburnt, this has burnt from here they said the heat transfer takes place due to the heat transfer.

So, burning takes place or the other case, the diffusion approaches that from here the active radical or atoms of species diffuse through the unburnt side. So, in reality what happens if diffusion of heat and active radicals both are essentially they are because when there is a burnt mixture from this side, in obvious situation, there will be heat transfer to the unburnt mixture and there will be also some transfer or the diffusion of the active radicals which will take part in the process.

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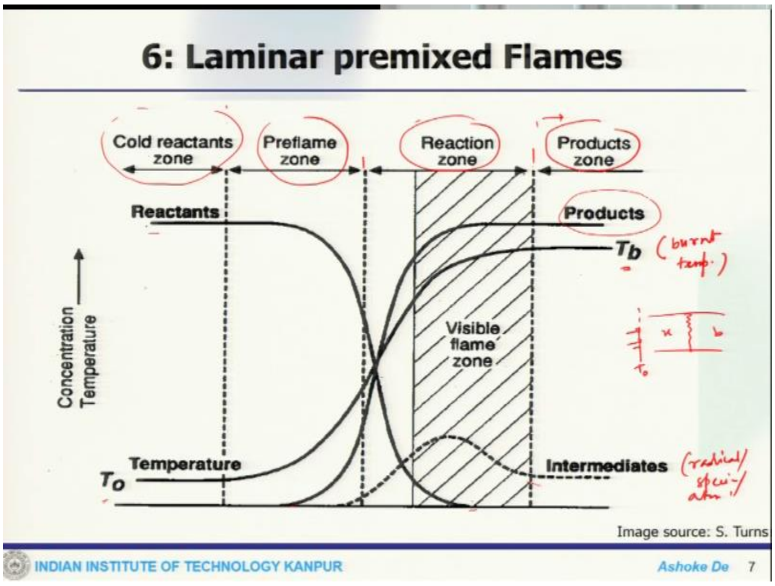

6: Laminar premixed Flames

Image source: S. Turns

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Now, this is a picture of a freely propagating premixed flame. So, this is very standard picture and available in any textbook and what it shows that that this is the initial mixture, which is at the lower temperature. So, as it goes along this reaches a final temperature this is your burnt temperature that means, the other side of the reaction zone, this is the flame thickness, this is my burnt side, this is uhburnt side and when the temperature goes up due to reaction, the reactions will also automatically gets consumed.

So, this is my starting point of the reactants at the initial stage and as it getting consumed, it will come down and it completely consumed. So, that is how happens to the reactants and one is the reactors reactants are getting consumed, obviously, we start getting the product. So, this is where the products so, one and so, this is very standard situation when there is a reaction zone, some reactants will be consumed, so, that concentration or mass would come down obviously, the product formation is there. So, that will go up.

Now, in between that there are some intermediates, these are intermediate this will be radical or species or atom whatever that form. Now, if you divide this whole picture, so, this side of this dotted line, this is a cold reactant zone that means here and this inner if this is my T_0 conditioned, so, this is all reactants are the cold condition. So, that means they are not getting into the business then as the things move along this particular zone called preflame zone quite slowly the reactants are getting heated up because of the temperature increase and all these.

And finally, this is that zone which is visible flame zone this whole zone from this dot to these called our reaction zone and in that reaction zone, you can see the abrupt changes of these reactant species which gets consumed completely, product species are formed, there is intermediate species which are also formed and the temperature goes up and finally this side of these product zones, because you have only the temperature of the burnt product and you get these things.

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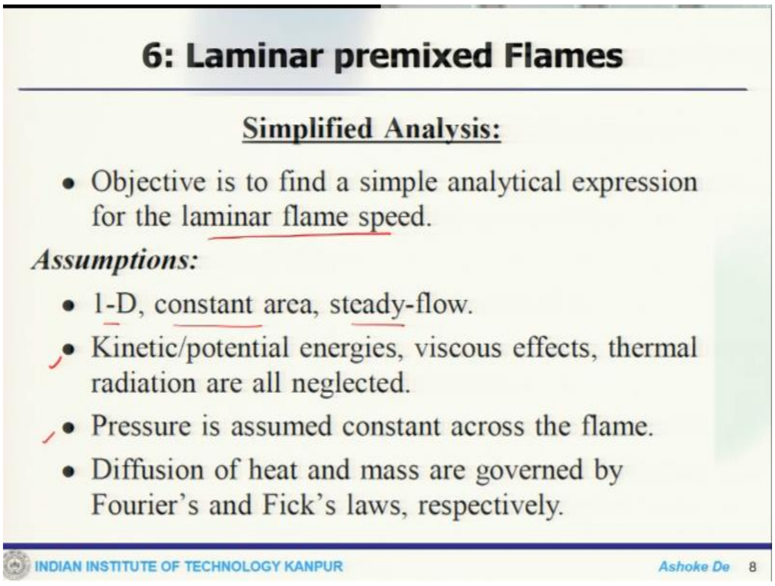

6: Laminar premixed Flames

Simplified Analysis:

- Objective is to find a simple analytical expression for the laminar flame speed.

Assumptions:

- 1-D, constant area, steady-flow.
- Kinetic/potential energies, viscous effects, thermal radiation are all neglected.
- Pressure is assumed constant across the flame.
- Diffusion of heat and mass are governed by Fourier's and Fick's laws, respectively.

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So, one can do some simplified analysis here. The whole idea is to find out the some simple analytical expression for the laminar flame speed or laminar burning velocity whatever you call it. So, to do that, any simplified analysis will obviously have some assumption first each 1-D constant area steady flow that is number one. So, then all your kinetic energies, potential energies, viscous effects and thermal radiation and these are all neglected.

So, that is number 2. Also across the flame, pressure is assumed to be constant. So, that means, there is no change in pressure or other pressure is not becoming an active parameter to contribute to that and diffusion of heat and mass, these are governed by the diffusion law like Fourier’s law and Fick’s law.

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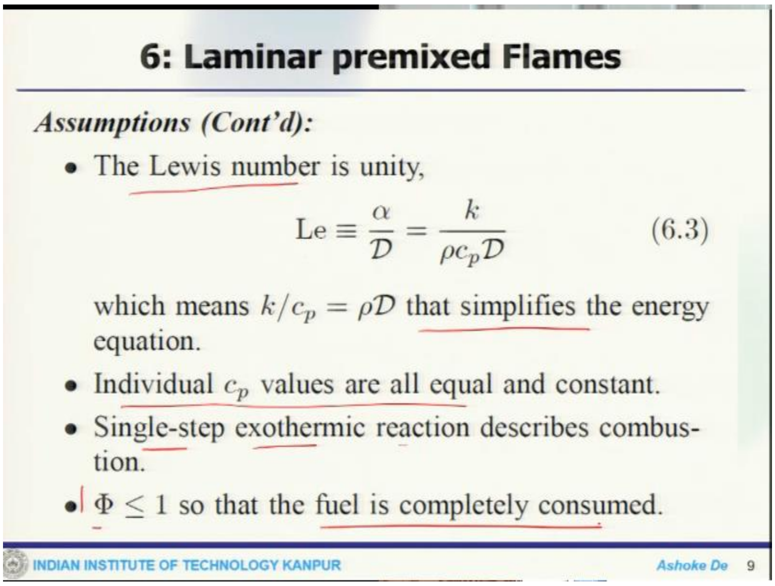

6: Laminar premixed Flames

Assumptions (Cont'd):

- The Lewis number is unity,

$$\mathrm{Le} \equiv \frac{\alpha}{\mathcal{D}} = \frac{k}{\rho c_p \mathcal{D}} \quad (6.3)$$

which means $k/c_p = \rho\mathcal{D}$ that simplifies the energy equation.

- Individual c_p values are all equal and constant.
- Single-step exothermic reaction describes combustion.
- $\Phi \leq 1$ so that the fuel is completely consumed.

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Then one more thing is a non dimensional number call Lewis number, which is the ratio between α and D is a thermal diffusivity to mass diffusivity or one can write in terms of:

$$Le = \frac{\alpha}{D} = \frac{k}{\rho c_p D}$$

So, the Lewis number is one that means, thermal diffusion and mass diffusion are occurring at the same rate. If it is one that means thermal diffusivity and mass diffusivity are of the same order. So, that where it helps because that simplifies the energy equation. Now, individual c_p values are all equal and constant.

So, if you take some species, the C p values are all equal and constant then kinetics which is important because when we are talking about the reaction and all these things, so, we have to take into consider the kinetics. So, this is a single step that means, it is a simplified already, which is essentially sort of in global kinetics exothermic reaction and we take a condition which is a lean condition that means the fuel is completely consumed. So, it is not a rich condition.

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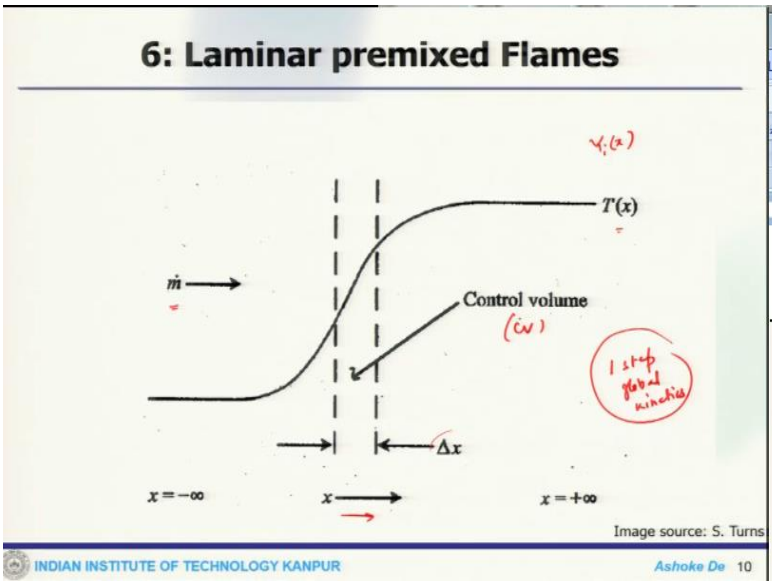

6: Laminar premixed Flames

Image source: S. Turns

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Now, if we look at the picture, so, this is how we define one dimensional. So, this is a one dimensional coordinate system, we take a small infinite small distance in that flame front that is Δx, this is the amount of reactant mass coming in. Essentially this is my control volume and this is the temperature rate. So, anything that we will get this will be all function of x only, because this is assumed to be one dimensional.

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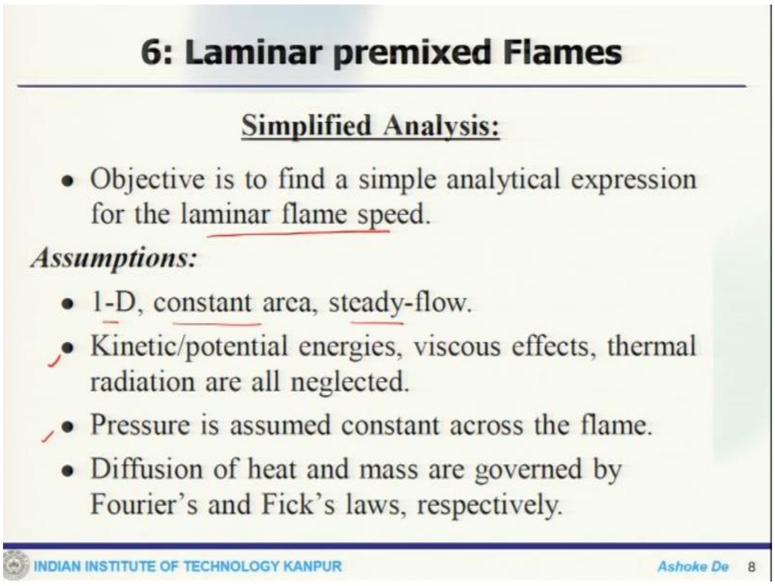

6: Laminar premixed Flames

Simplified Analysis:

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So, important conclusions are it is 1 D constant area steady flow, any other kinetic and potential energy these are neglected then, thermal diffusion and mass diffusion are occurring at the same rate and individual c_p values are equal and the reaction is 1 step global kinetics. So, that is how we define it. So, this is where we start our analysis. We will stop it here, and we will continue this analysis in the next lecture.