Turbulent Combustion: Theory and Modelling

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Lecture-41
Turbulence - Chemistry Interaction

Welcome back. So, let us continue the discussion on turbulence combustion. So far what we have covered we have looked at the fundamentals like basics, combustion then thermo dynamics, thermo chemistry and then we looked at the characteristics or properties of laminar flames like premixed flame or non premixed flame and then we had discussion on turbulence where we have seen how turbulent flow behaves.

And the scaling of the turbulent flows then the spectra and then we look at some of the modeling issues like what are the models which are available, how we actually use them. So, that is essentially provides you the platform to get into the actually turbulent reacting system, where we will be again looking at the system different system like turbulent premixed system, turbulent non premixed system, and how they interact to that turbulent environment.

So, it essentially burns down to him, you can think about it is turbulence chemistry interaction.

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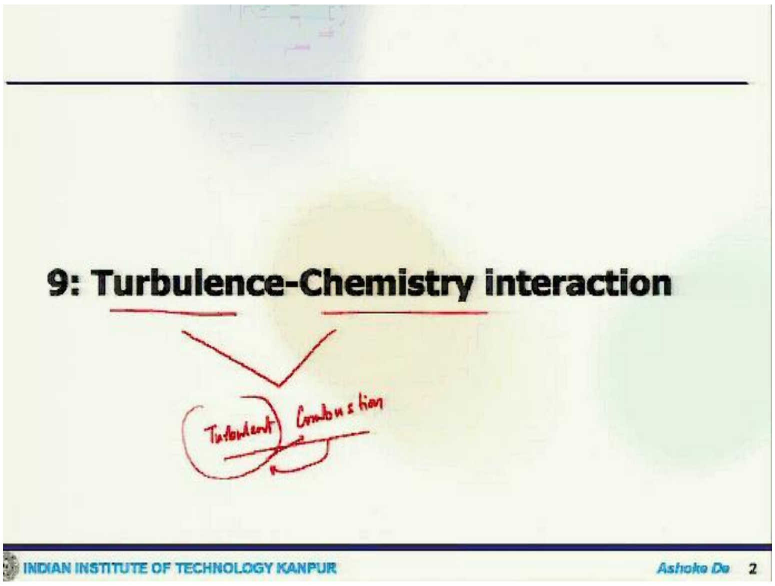

9: Turbulence-Chemistry interaction

Turbulent Combustion

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So, which talks if you need turbulent flow, you need chemistry. So, this in combinedly will give you all sort of turbulent combustion effect. So, the flow field is turbulent in nature that means the underlying field mechanics turbulent. So, it will essentially a random chaotic flame and then how that effect the reacting system at the same time, how the reacting system inversely effect the turbulent flow field. So, this is the combined effect that we want to look at in this turbulent chemistry interaction.

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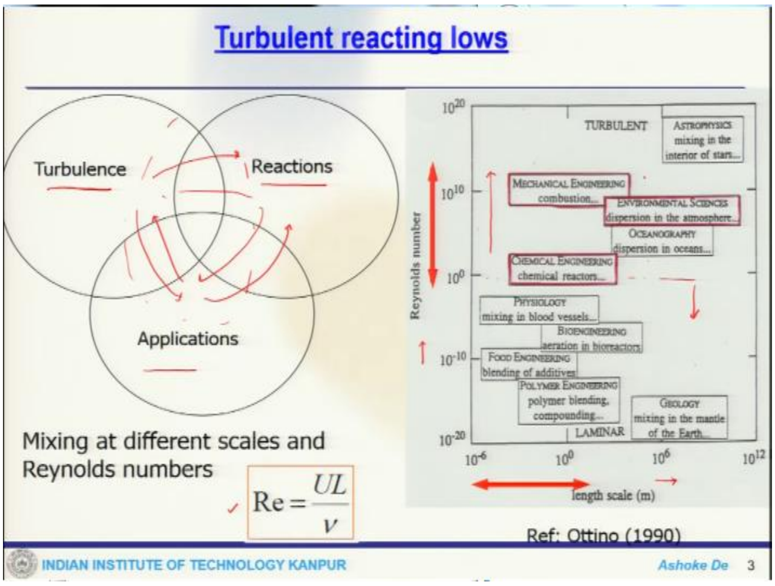

Turbulent reacting lows

Mixing at different scales and Reynolds numbers

$$Re = \frac{UL}{\nu}$$

Ref: Ottino (1990)

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So, to give an overview, this is what you can see this is where your turbulence is there and you have reactions and you have applications. So, they are sort of intersecting with each other and so, there would be mixing at different scale and we defined things by reynolds number. So, this intersection picture here it has the plenty of meaning, it tells you a lot of thing that things or it sends you a lot of message which exactly tells you that turbulence effect this effect turbulence, it effects applications also application effect reaction.

So, these are all sort of coupled phenomena and you cannot leave one from the other. Now, if you look at the range of the application, there is a wide range of application and this is in you, this axis, it is the length scale and this is the reynolds number. So, this is the laminar zone then once we start getting into so these below this line, these are laminar system, but chemical engineering or chemical reactors, oceanography, where the dispersion in oceans, environmental science, mechanical engineering all these.

This is the range where you actually see the impact of the large scale turbulence and if the system is reacting, then the interaction is huge.

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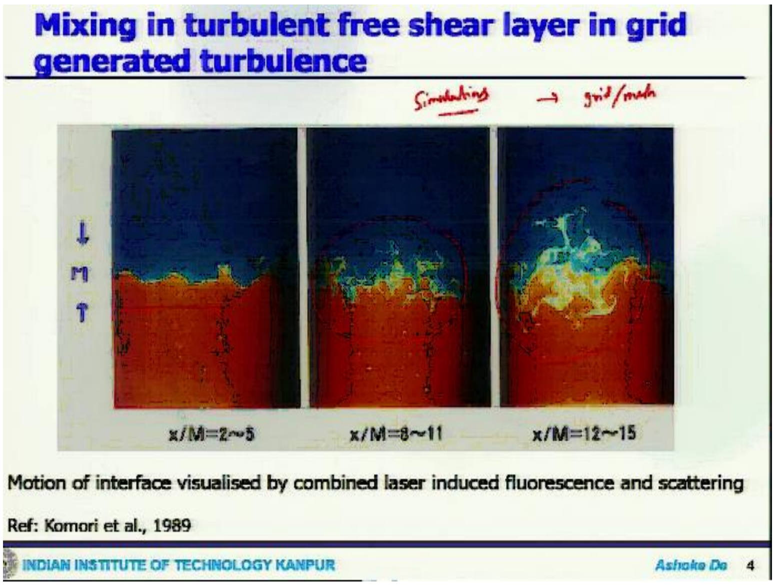

Mixing in turbulent free shear layer in grid generated turbulence

Simulations → grid/mesh

Motion of interface visualised by combined laser induced fluorescence and scattering

Ref: Komori et al., 1989

Now, this is another picture of mixing layer mixing in free shear layer, where the motion of the interface is visualized, you can see there is a structure here and there is a huge difference of the structure and this is more or lie chaotic in nature and this happens, this is happening in a simulation and simulations dependent on your grid or the maze, this is what you see in grid generated turbulence and this chaotic maze show in your result, but inherently you can absorb the flow field to be chaotic.

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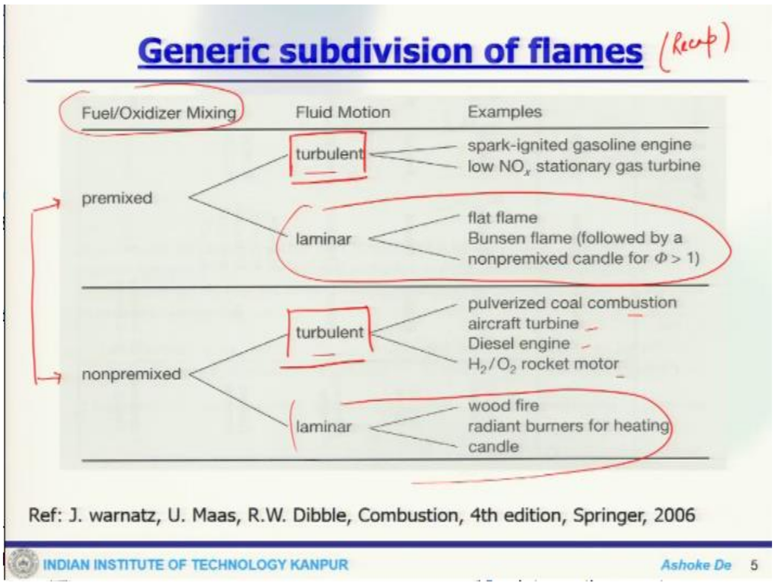

Generic subdivision of flames (Recap)

Fuel/Oxidizer Mixing	Fluid Motion	Examples
premixed	turbulent	spark-ignited gasoline engine low NO_x stationary gas turbine
	laminar	flat flame Bunsen flame (followed by a nonpremixed candle for $\Phi > 1$)
nonpremixed	turbulent	pulverized coal combustion aircraft turbine Diesel engine H_2/O_2 rocket motor
	laminar	wood fire radiant burners for heating candle

Ref: J. warnatz, U. Maas, R.W. Dibble, Combustion, 4th edition, Springer, 2006

Now, again just to recapitulate that thing this is what we have been talking again and again it is a depend on fuel and oxidizer mixing, we categorized them in 2 category one is the premixed, another is the non premixed, if it is turbulent, so, there could be spark ignitions in these gas turbine engine non premixed, if it is turbulent you have a coal combustion, aircraft, gas turbine, diesel engine, rocket motors.

So, laminar one already we have done the discussion on the laminar cases, so now we want to concentrate on turbulent premixed combustion and turbulent nonpremixed combustion and towards the end to talk about multi phase system.

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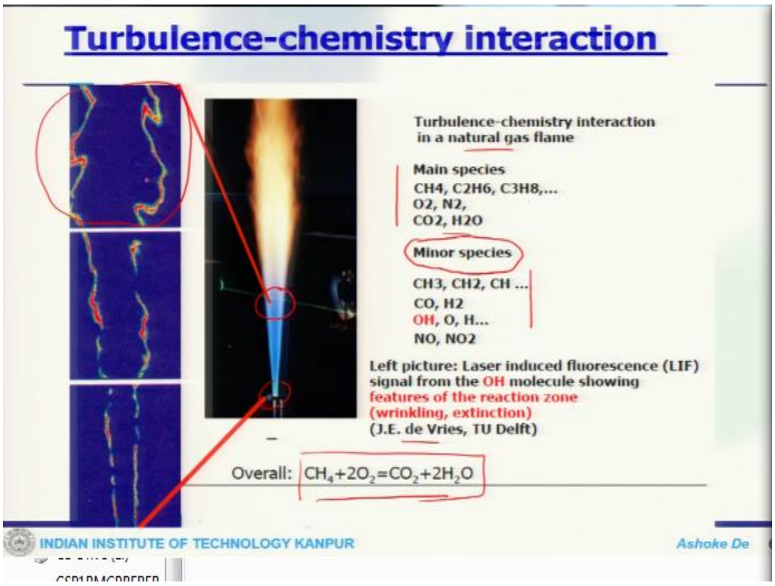

Turbulence-chemistry interaction

Turbulence-chemistry interaction in a natural gas flame

Main species
CH4, C2H6, C3H8,...
O2, N2,
CO2, H2O

Minor species
CH3, CH2, CH ...
CO, H2
OH, O, H...
NO, NO2

Left picture: Laser induced fluorescence (LIF) signal from the OH molecule showing features of the reaction zone (wrinkling, extinction)
(J.E. de Vries, TU Delft)

Overall: $CH_4+2O_2=CO_2+2H_2O$

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So, that is what for this is another picture which is obtained from this experiment where this is a laboratory scale burner, it is an unconfined flow or the unconfined jet, reactant jet you can so, this is the methane combustion. So, overall reaction you can think about in that methane burning with oxygen producing these.

So, it is a natural gas that is why we say there are major species which are CH_4, C_2H_6, O_2, N_2, CO_2, H_2O and there are minor species which are also involved in the reacting system like CH_3 and the importance of minor species has already been discussed in details when we talked about the kinetics and the impact of the kinetics that these are the species are radicals which are formed and they heat to propagate the reaction.

So, once we taken OH images and this is the OH image which shows the reaction zone and this picture corresponded to the position here spatial location this is at the here you can see that jet is coming out the free shear layer is nicely found and the shear layer found here because it is something which is distorted here you can see because of the small scale eddies or because of the turbulence the reaction is distorted or wrinkled or whatever we say. So, the impact of the turbulent flow field is clearly visible here.

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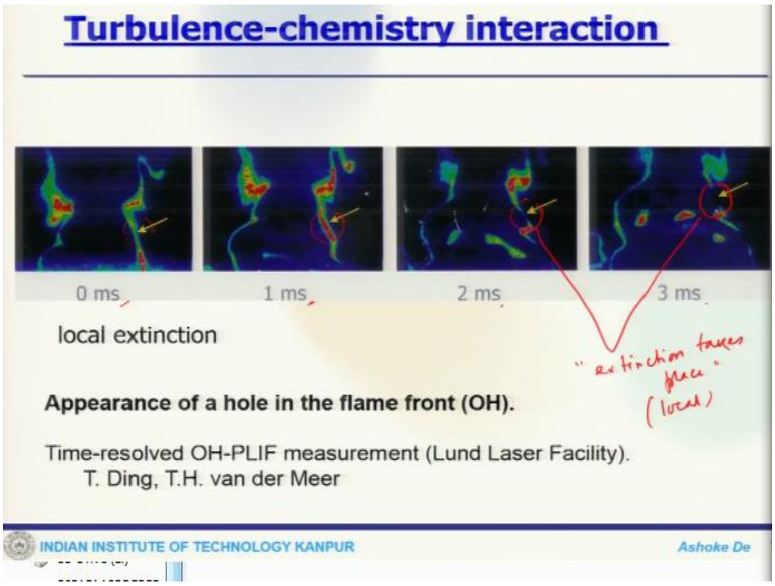

Turbulence-chemistry interaction

local extinction

" extinction takes place "
(local)

Appearance of a hole in the flame front (OH).

Time-resolved OH-PLIF measurement (Lund Laser Facility).
T. Ding, T.H. van der Meer

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Now, again the OH measurement for a banner, when you look at the reaction zone this is at a time of 0 millisecond, this is at 1 millisecond, this is at 2 milliseconds and 3 milliseconds what is so, that at this initial stage you can see it is a nice pattern of the flame then probably it becomes increasing the temperature, but some point they are you can see there is a hole in the flame front and this is clearly visible here. So, these are the situation when the extinction takes place.

So, this is not global extinction, this is rather local extinction because you can still see the flame front there that the under reaction zone, but this extension is in local extinction. So, that is also possible situation under and that happens because your flow field is turbulent. So, under turbulent condition, so, when the reaction zone on the flame front is reacting with them small scale eddies then you can have this kind of local extinction.

So, capturing or prediction of this kind of local extinction is also quite challenging.

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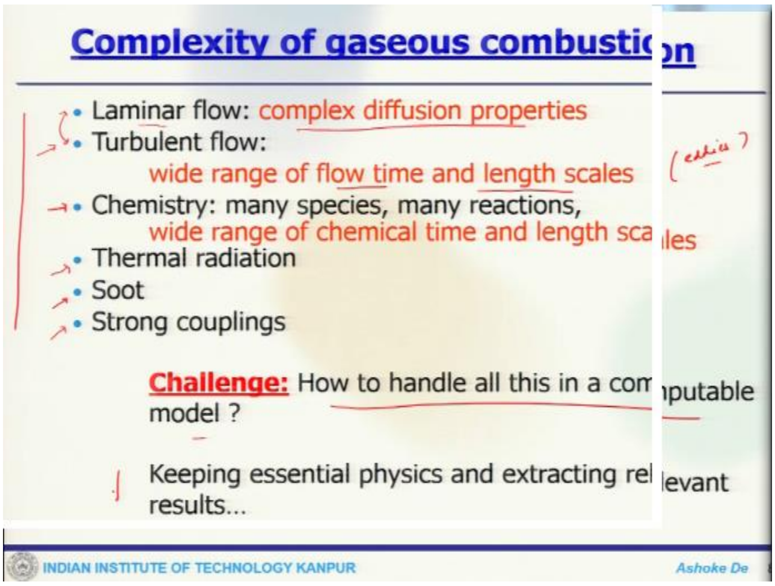

Complexity of gaseous combustion

- Laminar flow: complex diffusion properties
- Turbulent flow:
  wide range of flow time and length scales (eddies)
- Chemistry: many species, many reactions,
  wide range of chemical time and length scales
- Thermal radiation
- Soot
- Strong couplings

Challenge: How to handle all this in a computable model ?

Keeping essential physics and extracting relevant results...

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So, if you put things together in the context of gaseous combustion. So you have, if you the flow is laminar then you have complex diffusion properties, if the flow is turbulent then that immediately gives you wide range of flow time and length scales. So, that means, because of this eddies you have multiple length and timescale, so under, So, immediately you can see, one can compare these 2 situation laminar to turbulent and can see the immediate difference in the length and timescale and obviously, now, top of that you need chemistry.

So, there are multiple species they are involved in the reacting system. So, the timescale and length scale would be also wide range of length and timescale. So, that means, you have flow timescale you have kinetics timescale then, if you have some edit situation or edit feature, which are associated with that phenomena then you can have radiation it will have different time and length scale you have soot which you will have also different scale than the coupling with other physics.

So, the whole point is that how to handle all this in a computational model, because, if one has to look at in a computation field, then one has to look at it, but when you deal with all this, you have to keep one thing in mind that you cannot actually compromise on the physics. So, your results should be reasonable enough that it should not compromise on the physics.

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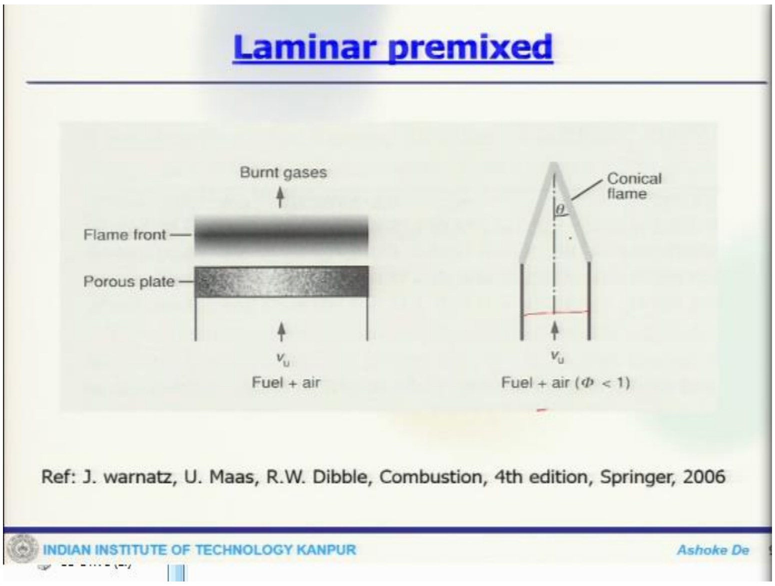

Laminar premixed

Ref: J. warnatz, U. Maas, R.W. Dibble, Combustion, 4th edition, Springer, 2006

So, this is a simple laminar premixed system which we have seen this is a conical flame, when it comes through these things where fuel and air here in condition, it burnt, you get conical flame like this and this is a flame front burnt simple gas.

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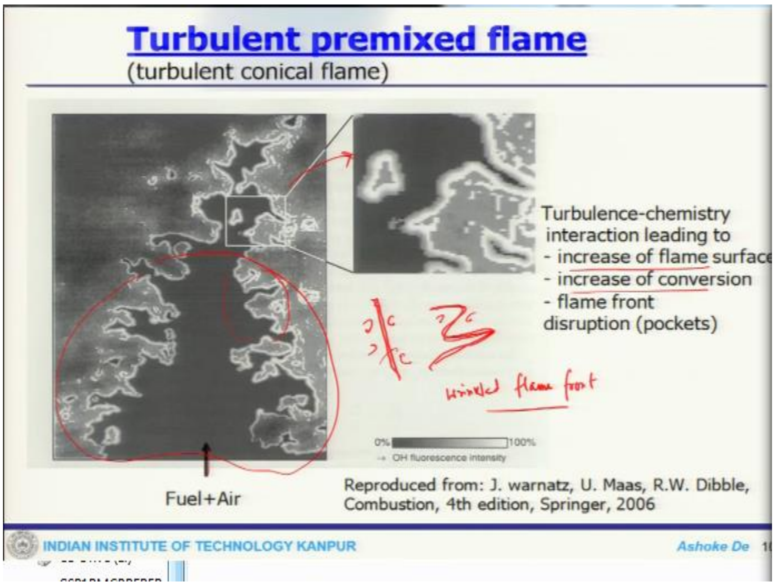

Turbulent premixed flame

(turbulent conical flame)

Turbulence-chemistry interaction leading to
- increase of flame surfac
- increase of conversion
- flame front disruption (pockets)

Reproduced from: J. warnatz, U. Maas, R.W. Dibble, Combustion, 4th edition, Springer, 2006

But at the same time, when you look at the situation under turbulent condition, so, these are the images from turbulent system. So, you see, huge this is the fuel air mixture coming and this is the conical and you can see the structure, this is your flame front essentially this portions are the flame front and the one of the position is zoomed and shown here. So, if you look at this flame front compared to the previous picture here, you see a huge difference and this difference primarily comes because your flow field is turbulent in nature.

So, that turbulent flow field has different range of scales that is a large scale, intermediate scale, small scale and smaller scales. So, they are interacting each of these small and small a different eddies of different size, they do interact with the flame front, if I have a flame front like this then this eddies will interact with that some eddies may penetrate some may not penetrate, so, they will actually have tremendous impact on the flame front and that is why you can get you get to see these kind of distorted flame front or rather sometimes you called it wrinkled flame front.

So, these are the very unique characteristics of turbulent system. So, what it does at the same time that because of this interaction process, it actually increases the surface area, now, thing is that my flame surface can be wrinkled like this, because of this eddies interaction. So, once you look at this effective surface area of the flame front that actually increases, so, it is increase the conversion of that, that means, more surface area means your volumetric utilize will also increase.

So, that will also at the same time disrupt the flame pockets, so it is one over other it is sort of a coupled system.

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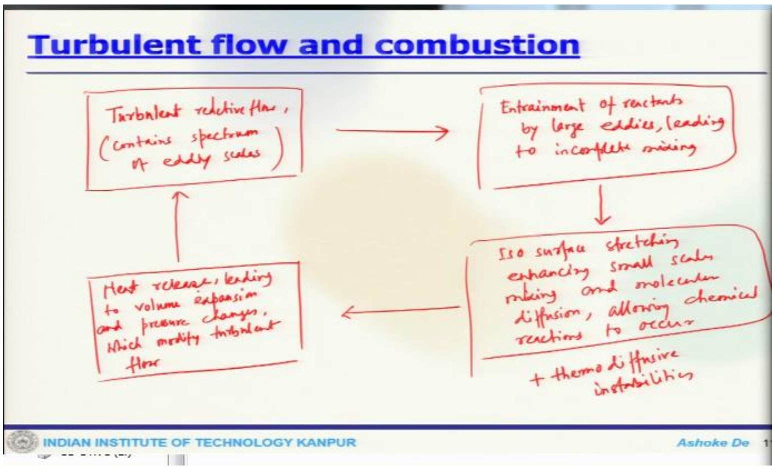

Turbulent flow and combustion

Turbulent reactive flow, (contains spectrum of eddy scales)

Entrainment of reactants by large eddies, leading to incomplete mixing

Iso surface stretching enhancing small scales mixing and molecular diffusion, allowing chemical reactions to occur

+ thermo diffusive instabilities

Heat release, leading to volume expansion and pressure changes, which modify turbulent flow

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Now, if you want to look at the combined effect one can put that okay this is my turbulent reactive flow so, which contains spectrum of eddy scales. So, one that have, so that will allow you to entrainment of reactants by large eddies which leading to incomplete mixing. So, this will you have different range of scales that will into then you have iso surface stretching enhancing the enhancing small scales or small scale mixing and molecular diffusion allowing chemical reaction to take place, allowing chemical reaction to occur.

So, that essentially So, this can add to also thermo, diffusive, instabilities So, that would go to heat release which will lead to volume expansion and researching this which modify turbulent flow so, that again in turn have the impact on the reacting system. So, if you look at this complete picture this essentially becomes a kind of closed loop you may have in fact turbulent reacting system.

So, you have large range of skills because of the eddies they allow mixing large scale it is react to differently compared to small scale it is then your iso surface stretches it helps in small scale mixing and your reaction to take place once you have reaction to take place you have a volumetric heat release. So, due to volumetric heat release your pressure changes. So, also the local momentum changes in term it changes the local behavior of the turbulent flow.

So, it is an, so one hand turbulent effecting the reaction other hand reaction effecting the turbulent, it is a sort of a hand shaking, so becomes quite complicated because of different scales we see there.

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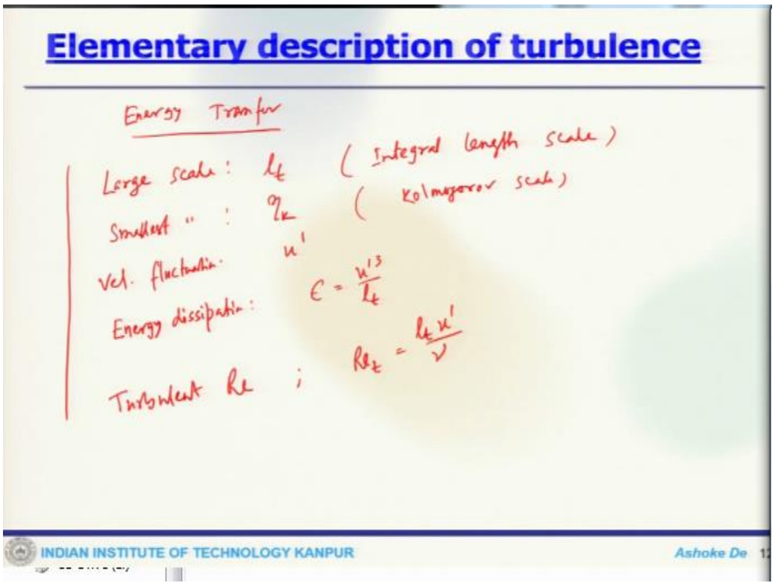

Elementary description of turbulence

Energy Transfer

Large scale : l_t (Integral length scale)

Smallest " : η_k (Kolmogorov scale)

Vel. fluctuation: u'

Energy dissipation : $\epsilon = \frac{u'^3}{l_t}$

Turbulent Re ; $Re_t = \frac{l_t u'}{\nu}$

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Now, just in, some of the description which we have already looked at. So, energy transfer that is one thing or important phenomena here from large scale to small scale the energy transfer takes place and at the smallest scale which is kolmogorov scale. So, that is dissipated then the scale, so we can say define the large scale of l_t which is also integral length scale then the smallest scale would be η_k which is Kolmogorov scale and then velocity fluctuation standard deviation.

And velocity fluctuations which will be u prime energy dissipation which is epsilon power by l_t and turbulent Reynolds number which is defined as

$$Re_t = \frac{u' l_t}{\nu}$$

and all these issues with these things like the scales and all these we have already done detailed discussion during turbulence and all this, this is just to recap because we are going to use these scales when you talk about these different aspect.

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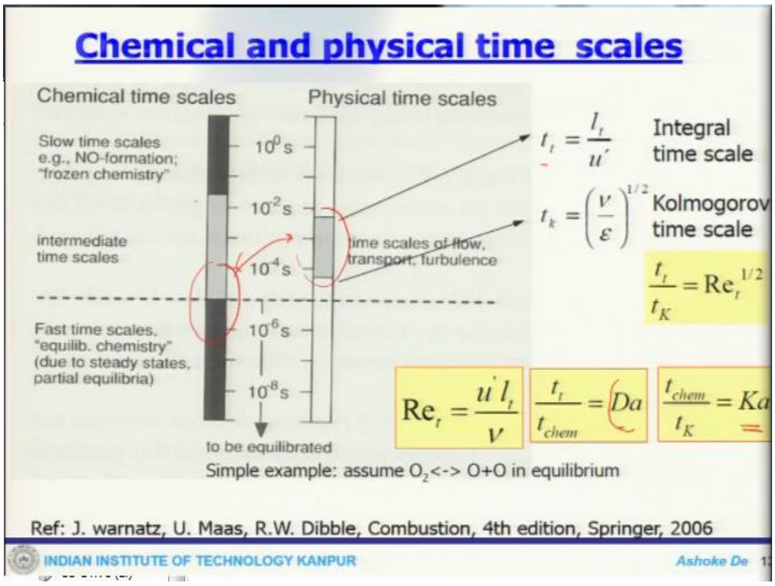

Chemical and physical time scales

$t_t = \frac{l_t}{u'}$ Integral time scale

$t_k = \left(\frac{\nu}{\varepsilon}\right)^{1/2}$ Kolmogorov time scale

$\frac{t_t}{t_K} = \mathrm{Re}_t^{1/2}$

$\mathrm{Re}_t = \frac{u' l_t}{\nu}$ $\frac{t_t}{t_{chem}} = Da$ $\frac{t_{chem}}{t_K} = Ka$

Simple example: assume O_2<-> O+O in equilibrium

Ref: J. warnatz, U. Maas, R.W. Dibble, Combustion, 4th edition, Springer, 2006

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Now, one quick thing to go through is the different time scale. Now, typically, this is where your physical time scale or the flow time scale that is there and you can define your integral timescale like is in l_t/u' and the kolmogorov time scale would be $\left(\frac{\nu}{\varepsilon}\right)^{1/2}$, so the issue of these 2 timescale would be $Re_t^{1/2}$ and Re_t one can define $\frac{u' l_t}{\nu}$, the other hand when you look at the chemical timescale, they are quite different like if you have equilibrium chemistry.

So, they will belong in these there will be some intermediate time scale and there is it a slow forming species like frozen chemistry are enormous and they will have this timescale. So, there is a range of scale especially under chemical timescale, there is a variation, that variation gives and, or opens upon challenge that the flow timescale may be here and reacting time scale may lie here, how to manage these gap because there is a gap.

So, that is the whole point of discussion and we will discuss theoretically and also then look at the aspect of the modeling point of view, how we managed to batch of this gap. So, now, if you have a chemical timescale and there is a flow timescale, integrals time scale that ratio called the damkohler number, which is a non dimensional number and the chemical timescale to kolmogorov that is the kolmogorov number. So, these are the non dimensional number that is what going to be used to carry some of these scales.

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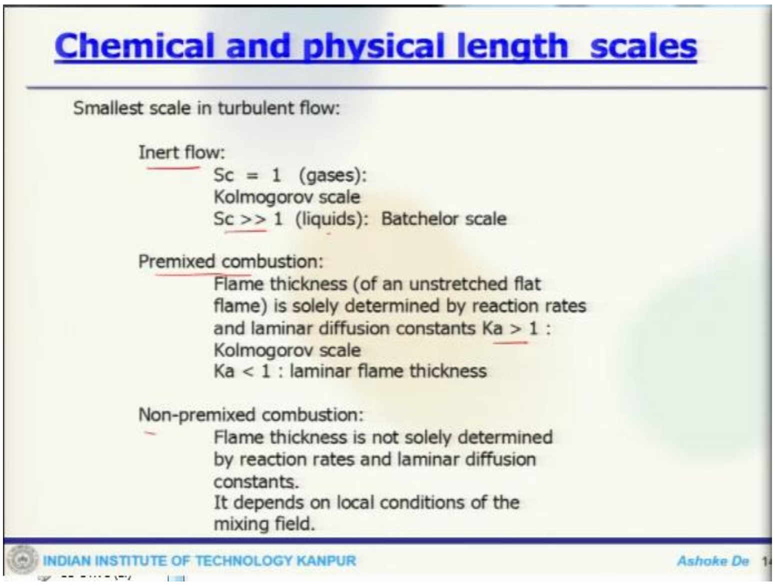

Chemical and physical length scales

Smallest scale in turbulent flow:

Inert flow:
- Sc = 1 (gases):
  Kolmogorov scale
- Sc >> 1 (liquids): Batchelor scale

Premixed combustion:
- Flame thickness (of an unstretched flat flame) is solely determined by reaction rates and laminar diffusion constants Ka > 1 :
  Kolmogorov scale
- Ka < 1 : laminar flame thickness

Non-premixed combustion:
- Flame thickness is not solely determined by reaction rates and laminar diffusion constants.
- It depends on local conditions of the mixing field.

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Now, if you look at these scales inert flow, Schmidt number is 1 and Kolmogorov scale Schmidt number would be quite high for liquids. Now, when you look at the previous combustion, the flame thickness is surely determined by the reaction rate and laminar diffusion constant. So, the kolmogorov number would be greater than 1 and it kolmogorov at the kolmogorov scale kolmogorov number is less than 1 where you go to non premixed system flame thickness is not solely determined by the reaction rate.

It is a laminar diffusion constant it rather depends on local condition of the mixing field.

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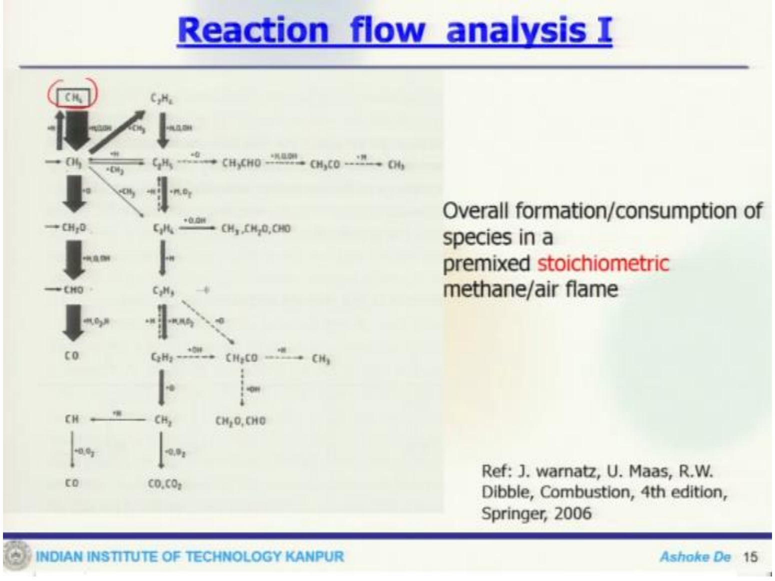

Reaction flow analysis I

Overall formation/consumption of species in a premixed stoichiometric methane/air flame

Ref: J. warnatz, U. Maas, R.W. Dibble, Combustion, 4th edition, Springer, 2006

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So, you can see this how this reaction patterns actually or reaction pattern takes place this is a natural gas combustion already we are talking about the thermo chemistry we got an idea about, so that forms some CH_3 radicals, CH_2O, CHO, CO and then it expands. So overall formation or consumption of species in a premixed stoichiometric. So, this goes through multiple branching.

So that is why we have seen the change in the phase and reaction, change propagation reaction and finally the change dimension because radicals are form in between.

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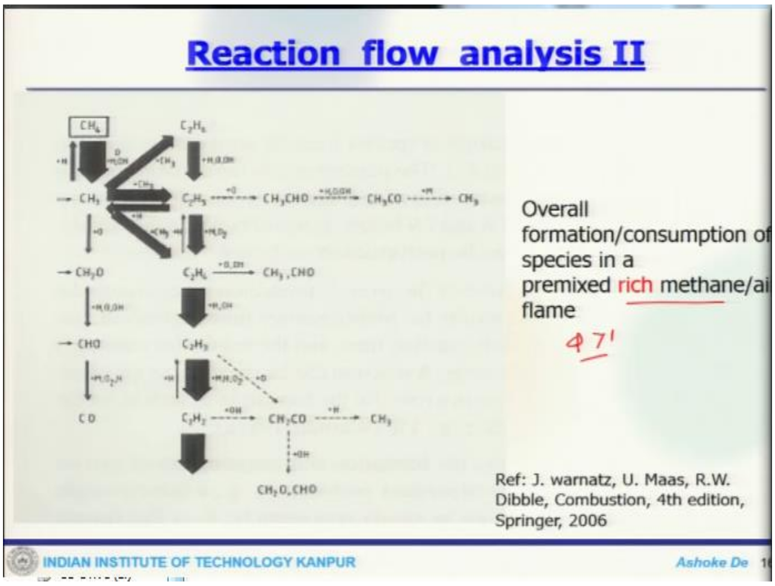

Reaction flow analysis II

Overall formation/consumption of species in a premixed rich methane/ai flame

47'

Ref: J. warnatz, U. Maas, R.W. Dibble, Combustion, 4th edition, Springer, 2006

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And they actually allow to this is a situation when you have a rich methane air flame that means the equals issue is more than one and they are the intermediate species formations are quite different. But though there would be species formation, because otherwise that without the species formation the reaction cannot propagate. So, that should be there.

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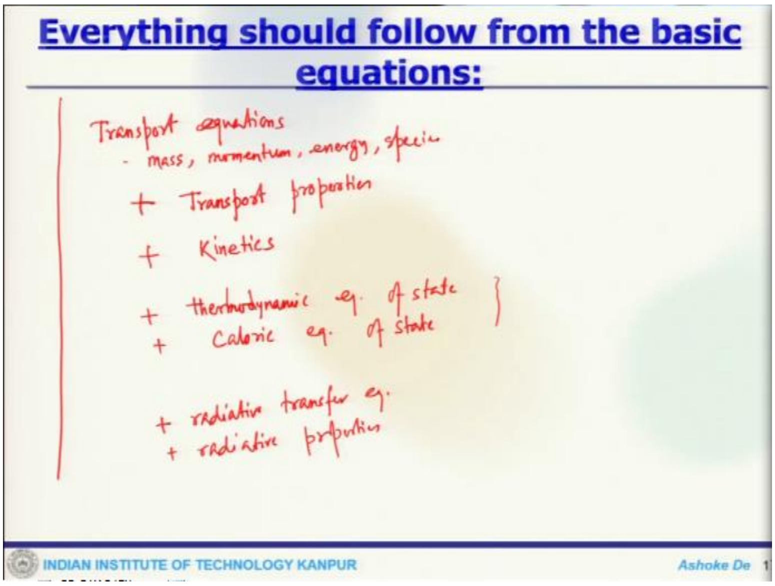

Everything should follow from the basic equations:

Transport equations
- mass, momentum, energy, specie

+ Transport properties
+ Kinetics
+ thermodynamic eq. of state }
+ Caloric eq. of state
+ radiative transfer eq.
+ radiative properties

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Now, if we put everything together, and when we try to define this reacting system under turbulent condition, so, we need some governing equations. So, first thing that we need is that all that transport equations so, that will have mass, momentum, energy and species. So, these are the state of governing equations or the transport equation that one needs to define the system plus we need transport properties.

So, these are also important transport properties like viscosity, diffusivity, thermal conductivity like that, then this can define the flow field we need kinetics, which is required to represent the reacting system then we need thermo dynamic equation of state and caloric equation of state so, that will allow you to calculate properties and all those things then, if you have radiation then we need a radiative transfer equation which we need radiative properties. So, this is the state of equation.

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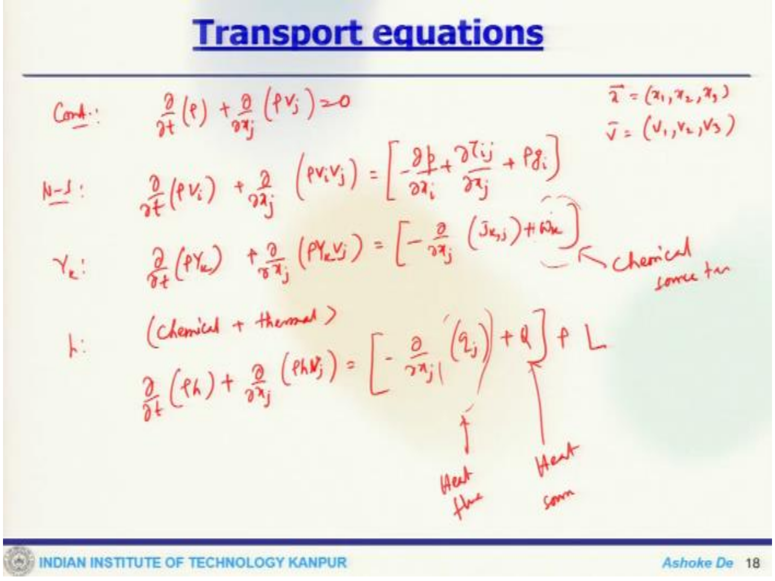

Transport equations

Cont.: $\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_j}(\rho v_j) = 0$

$\vec{x} = (x_1, x_2, x_3)$

$\vec{v} = (v_1, v_2, v_3)$

N-S: $\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_j}(\rho v_i v_j) = \left[-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i\right]$

Y_k: $\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_j}(\rho Y_k v_j) = \left[-\frac{\partial}{\partial x_j}(J_{k,j}) + \omega_k\right]$ ← Chemical source term

h: (chemical + thermal)

$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_j}(\rho h v_j) = \left[-\frac{\partial}{\partial x_j}(q_j) + Q\right] + L$

Heat flux

Heat source

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So, the quickly to get to the transport equation, we can say this is our x_1, x_2, x_3 and velocity component would be v_1, v_2, v_3. So, our continuity is

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_j}(\rho v_j) = 0$$

Momentum of the Navier Stokes for

$$\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial t}(\rho v_i v_j) = \left[-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i\right]$$

So the Y_k is the species mass transfer equation. So, we can write

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_j}(\rho Y_k v_j) = \left[-\frac{\partial}{\partial x_j}(J_{k,j}) + \omega_k\right]$$

and enthalpy equation that specific enthalpy which is sum of chemical plus thermal.
Which will be

$$\frac{\partial}{\partial t}(\rho_h) + \frac{\partial}{\partial x_j}(\rho_h v_j) = \left[-\frac{\partial}{\partial x_j}(q_j) + Q\right] + L$$

So, now, this term is a chemical source term, this is the term heat flux, this is heat flux, this is heat source, this is chemical source term. So, these are the state of equations that you need. So, stop here today and continue the discussion in next lecture.