Turbulent Combustion: Theory and Modelling Prof. Ashoke De Department of Aerospace Engineering Indian Institute of Technology – Kanpur

Lecture - 49 Turbulence- Chemistry Interaction (contd…)

Welcome back. So, let us continue the discussion on different combustion modeling approaches and they are theoretical as well as the numerical point of view. So, what we have done so far we have looked at the simple models like started with Eddie breakup model the eddy dissipation model and then followed by a discussion on the eddy dissipation and combustion model and then we have looked at the statistical-based model like transported PDF. So, now, we will move to the next set of discussions.

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Which will be specific or rather more applicable to the premixed combustion and that context we will discuss some of this premixed combustion based model. So, what we have done so far we have discussed this part, which applies to any mode of combustion, though, have already mentioned anything applicable means does not become it is going to be accurate enough but they can be theoretically applied to any set of the model with their pros and cons are these set of models are very specific to the premixed combustion. Then we will go to the non-premixed combustion.

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So, just to quickly look at the freely propagating premixed flame this is what we see your reactant comes in we have the product and this is going to be reaction zone where your chemical reaction takes place, because of that, there would be heat release and there will be density change and the flow excellent. One of the very fundamental properties of the premixed flame is their velocity or laminar flame velocity or laminar burning speed and the second one is the flame thickness.

So, if you just recall this laminar flame speed or laminar burning velocity proportional to the diffusivity, and also the chemical timescale.

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Model equations steady 1D premixed flame
\nContinuity
\n
$$
\dot{M} = \rho u = const.
$$
\nSpecifices mass fractions
\n
$$
\dot{M} \frac{d}{dx} Y_k + \frac{d}{dx} (\rho Y_k V_k) = \omega_0 \hat{N} \hat{k} = 1, \dots, N-1
$$
\nTemperature
\n
$$
C_p \dot{M} \frac{d}{dx} T = \frac{d}{dx} \left(\lambda \frac{d}{dx} T \right) - \sum_{k=1}^{N} \rho Y_k V_k C_{p,k} \frac{d}{dx} T + \sum_{k=1}^{N} \omega_k h_k
$$
\nEquations of state
\n
$$
\rho = \frac{p \overline{W}}{R_u T} \qquad h_k = \Delta h_{f,k}^0 + \int_{T_0}^{T} C_{p,k} (T') dT'
$$

So, now, for this freely propagating system, this will be one-dimensional premixed flame, so, we have our continuity equation. Then, we write them species mass fractions equation where this is the chemical source term as we have seen it so many times chemical source term and then we write the temperature equation this is specifically for this freely propagating flame which does not sound that remains one dimensional in variation.

So, we like the temperature equation there, and then to close down all these above equations, we require an equation of state, where pressure, density are coupled and then the enthalpy which has the enthalpy formation and the other part.

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So, now, one of the things which is required is the diffusivity of the species, for the time being, will assume the constant Lewis number model. So, that means Lewis number is 1 typically if you look at that for different species, this is how the various of the Lewis number and now, once you assume the Lewis number 1 So, that means your thermal diffusion and mass diffusion they will be of the same order.

So we will use Fick's law of diffusion, which we right in terms of gradient and then we get the relationship between λ and C_p which is in temperature dependency there.

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Now, we convert the temperature equation and if we plot these things for the different term in the reaction zone, there is always a balance between convection and conduction that means, this is the term and this term and reaction zone this should be I mean this is sorry preheat zone and this side is the reaction zone. So, this is a balance between reaction conduction and convection and these are the different terms for to you can plot and see how they vary from one zone to another zone.

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So this picture we have seen it what happens in a turbulent flame front you see a lot of wrinkles like this and this is because of your eddies and these eddies can allow these flames surface to wrinkle like that so this turbulent chemistry leading to increase of flame surface to increase our conversion that means heat release will increase flame front disruptor. So that this will not only increase the surface in the while there is increasing the surface volumetric heat will increase at the same time there could be some disruption of the flame front.

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Now, just to a quick recap of the this is how one can see the structure of premixed flames. I mean these are turbulent premixed flames, and you can see different kind of structure all these wrinkled or the curved wrinkles shape is primarily due to eddy's of different scale, which could be starting from the large scale to small scale. So multiple-scale that would form that.

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Now, if you look at the instantaneous images, this is the instantaneous frame front what you can see and if you put that flame brush, this is what one can see, I mean this is the flame brush and in between, there will be a lot of this chaotic random less.

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Turbulent premixed Flames

- · Definitions:
- Laminar flame thickness:

$$
\delta_L \sim \alpha / S_L = D / S_L = \nu / S_L \tag{1}
$$

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- Above equality implies that we assumed, Schmidt Number: Sc = $\nu/D = 1$ Lewis Number: Le = $\alpha/D = 1$ Prandtl Number: Pr = $\nu/\alpha = 1$

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So, one is the definition of the flame thickness which is

$$
\delta_L \sim \frac{\alpha}{S_L} = \frac{D}{S_L} = \frac{v}{S_L}
$$

One can write in terms of diffusivity and the flame speed Schmidt number which is 1, Lewis number is 1, Prandtl number is 1. These are the non-dimensional numbers.

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Now, there would be one important definition which is required to the turbulent Reynolds number, this turbulent Reynolds number is defined as u prime lambda by nu where lambda is the integral length scale of the turbulence. So, that turbulent Damkohler number will be a ratio of the flow timescale to chemical timescale. So, this will dictate which one is dominating whether the flow is dominating or the kinetics is dominating.

So, depending on that, so, the Damkohler number would play an important role and one can distinguish different flame zones to that.

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The flow timescale would be

$$
\tau_{flow} = \Lambda/u'
$$

Λ is our integral length scale. Characteristics timescale is

$$
\tau_c = \delta_L / S_L
$$

So, the Damkohler number is a ratio of flow timescale to chemical timescale.

$$
Da = \frac{S_L \Lambda}{u' \delta_L}
$$

So, once you put that, this is what you get this lambda if we now use the Taylor microscale and Kolmogorov length scale.

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We can use that thing to define the Karlovitz number which is

$$
Ka = \left(\frac{\Lambda}{\eta}\right)^2 = \frac{\delta_L u'}{S_L \lambda}
$$

So, one can write in terms of Taylor micro scale and fluctuating component of these things. So, the Reynolds number based on λ would be

$$
Re_{\lambda}=\frac{u'\lambda}{\nu}
$$

and turbulent Reynolds number based on η would be

$$
Re_{\eta}=u'\eta/v
$$

So,

$$
Re_{\Lambda} \approx Re_{\lambda}^2 \approx Re_{\eta}^4
$$

It is an important correlation one can think of that how the scale changes.

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Now, when there is a premixed flame front, one thing that will happen now, you will get one more important thing is that we have seen instead of laminar burn I mean top of the laminar burning velocity you get turbulent burning velocity. So, turbulent burning. So, this depends on the local mean property that is one of the important things but there is no consensus in literature heard that the burning velocity is a characteristic quantity that can be defined unambiguously for different geometries.

So that is another important point that means flame structure changes and the frame structure is also dependent on your turbulent scale, length scale, and timescale. Now, the turbulent length scale will also logical structure depends on the geometry. So, the large scale structure will react to the impact or would impact the flame front differently compared to a different length scale and the flame surface the formation would be different. So, that way these things are not very unique.

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Then, so, this was proposed by Damkohler, so there is the magnitude of the scale and then these

things so, we can have wrinkle flame or purely kinematically controlled flame.

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This is a simple structure where you have a flame front this is your unburned mixture and this is the burned mixture. So, the laminar flame velocity moves like this and if I take the surface this is how the turbulent flame front would be acting.

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Turbulent premixed Flames

- Damköhler equated the mass flux \dot{m} through the instantaneous turbulent flame surface area A_T with the mass flux through the cross-sectional area A_o . He used S_L for mass flux through A_T , and S_T for mass flux through A. $\dot{m}=\rho_u S_L A_T=\rho_u S_T A_o$ (8) $\frac{S_T}{S_L} = \frac{A_T}{A_o}$ (9) **A MOIAN WETTUTE OF TECHNOLOGY KANPUR**

So, through the equating the mass flux through the instantaneous turbulent flame surface area so, where we can write

$$
\dot{m} = \rho_u S_L A_T = \rho_u S_L A_o
$$

So, we are equating the mass flux whatever coming in that is going out and using that were adding that. So,

$$
\frac{S_T}{S_L} = \frac{A_T}{A_o}
$$

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Now, using the geometric approximation Damkohler proposed that this should be

$$
\frac{S_T}{S_L} = 1 + \frac{u'}{S_L}
$$

So, this is a very important correlation initial days people have used it extensively, but later on there are modification which are proposed to these kind of correlations.

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And one can also like Schelkin showed that this is not the linear variation of u'/S_L , it is something like and this so that short and relationship proposed by Klimov is something different which is

$$
\frac{S_T}{S_L} = 3.5 \left(\frac{u'}{S_L}\right)^{0.7}
$$

So, if you use different ratio of $\frac{S_T}{S_L}$, the impact on the flame front would be also different. So, these are the proposition that was made.

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Then later on Clavin and Williams proposed that no $\frac{S_T}{S_L}$ would be a different order. So, it is slightly more complicated and Gulder proposed that this would be of the disorder. So there are if you look at the literature, I mean, not only the textbook also the scientific reports and journals, you can see that there are plenty of these kinds of things, which are proposed and every correlation has its own advantage or disadvantage or rather proposed based on some set of observations or database which has collected due to that.

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What it essentially means that $\frac{S_T}{S_L}$ proportional to diffusivity, turbulent diffusivity, and molecular diffusivity. So, we can use that, but the turbulent diffusivity is proportional to this moleculer diffusivity. So, we can say that $\frac{S_T}{S_L}$ be proportional to like that.

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Now, if you have small intensity turbulence conditions, there are not many formulas and available so in this case that mixing is rapid as compared to the chemistry so and the distributed reaction zone Gulder in 1990 proposed that this ratio would be

$$
\frac{S_T}{S_L} = 6.4 \left(\frac{S_L}{u'}\right)^{3/4}
$$

SSo, as I said, these are there are multiple of this.

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But the situation is that the statement of the correlation of turbulent burning velocity is not universal or uniform. So, you require numerical simulation, I mean that is why using flamelet model turbulent burning closure direct numerical simulation, these are the things one has to do or look at typically.

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The experimental measurement methods they look at the conical stationary flames swelling flames and all these things were.

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So, now, if you look at the method of analysis, one way would be it is a flame normal analysis where you gather the information is that the extent to the flame surface or you can use the one point analysis. So, the flamelet based model these are will be the flame normal kind of analysis where you have a fresh gas and burnt gas and PDF models are essentially the one point analysis. **(Refer Slide Time: 14:04)**

So, when you do the flame normal analysis, there one important variable which is shown is that progress variable c, which is typically in fresh gas 1 and when it is the burnt gas it is a 0 and burnt get it is 1. So, these progress variables say that it is monotonously increasing from reactants to product side and it is normalized between 0 and 1. So, it could be defined in terms of species mass fraction or temperature like that.

Now, in the flamelet model, in turbulent calculations that transport equation of the progress variable is solved So, that means, along with our mass, momentum, turbulence, turbulence we solve also progress variable and then use the other information from the lookup table and all this we can solve for the rest of the things.

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Now we can typically for the premixed flame, there are different regimes one can. So, if you look at a simple one flame front which is reactants this side and products this is our laminar burning velocity, this is the flame thickness. So,

$$
\frac{u'}{s_L^o} = \frac{RMS \ velocity \ fluctuation}{laminar \ flame \ speed}
$$

$$
\frac{l_l}{\delta_L} = \frac{Integral \ length \ scale}{laminar \ flame \ thickness}
$$

So,

$$
\tau_{chem} = \tau_L = \frac{\delta_L}{s_L^o}
$$

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So, there are some other scales, one is you can have mean flow scale, well length scale is L/U, time is l_0/v and Kolmogorov scale it would be this and they are you have flame speed, flame thickness and all these.

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So, this is again important. We come back to this structure where your flow scale will be like this and then you will chemicals timescale is $\frac{\delta_L}{s_L^0}$. So, you can you need these to be connected with these turbulence Reynolds number, Damkohler number. So, the chemical timescale and the flow timescale they are sort of now.

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Some interpretation you can have a let us say planar of flame for uniform flow field is coming in like this. So, this would be our S_L this is a planar flame. So, the planar flame for the stability criteria is you have to be S_L then if you have let us say wrinkle flame this is our flame front. I will in the upcoming flow field which is coming at you. This is wrinkled flame and this is our SL.

So which is nothing but one can say the equivalence that you have some eddies like these small eddies which is interacting and then plus you have some flow. So there is a combination of these. So these are our eddies, so these combinations can give you this scale.

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So let us say if you have a situation like this, where this is the size and this is the length of the eddy L and this is my U_1 this is unburned and burned side then eddy size is 1, eddy velocity would be U_1 then turn over time would be eddy turn over time t eddy is $1/U_1$. So, the mixing time would be t_{mixing} would be l_k/u_k then we can find out this t_{eddy}/t_{mixing} is $Re_l^{1/2}$ where l_k is η and u_k is u_n that means Kolmogorov scale.

Physical interpretation of length, time and velocity scales INDIAN INSTITUTE OF TECHNOLOGY KANPUR

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Now you can have this kind of schematic like small structure to this goes too small and this goes to, so you have a inlet then this is your energy transfer. This already we have discussed in details it called is epsilon and this is in terms of heat. So, if you say this is my demarcation zone and this is my eddy size l, this would be my delta l that means the reaction zone. So, one can define the scale relationship among the scales.

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Like we can have ε which we have already seen, which would be

$$
\varepsilon \propto \frac{U_o^3}{l_o} \propto \frac{U_\eta^3}{\eta} \implies \frac{\tau_o}{\tau_\eta} \propto \left(\frac{l_o}{\eta}\right)^{2/3}
$$

Similarly

$$
\frac{U_{\eta}\eta}{\nu}\propto 1 \Longrightarrow \frac{\nu_{o}l_{o}}{U_{\eta}\eta} \propto Re_{l_{o}}
$$

Similarly

$$
\frac{l_o}{\eta} \propto \frac{v_o l_o}{\nu} \left(\frac{\eta}{l_o}\right)^{1/3}
$$

So, that is

$$
\frac{l_o}{\eta} \propto Re_{l_o}^{\frac{3}{4}}, \frac{U_o}{U_{\eta}} \propto Re_{l_o}^{1/4}
$$

and

$$
\frac{\tau_o}{\tau_\eta} \propto Re_{l_o}^{1/2}
$$

So, these relationships anyway this is a recapitulation because in the turbulent discussion we have done that.

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Non-dimensional numbers
\n
$$
h_{1b} = \frac{v_{1b}}{v} = \frac{v_{1b}}{v_{1b}}
$$
\n
$$
p_{1a} = \frac{v_{1a}}{r_c} = \frac{v_{1a}}{v_{1a}} = \frac{v_{1a}}{v_{1a}} = \frac{v_{1a}}{v_{1a}} = \left(\frac{v_{1a}}{v_{1a}}\right)^{-1}
$$
\n
$$
v_{1a} = \frac{v_{1a}}{r_{1a}} = \frac{v_{1a}}{v_{1a}} = \frac{v_{1a}}{v_{1a}} = \frac{v_{1a}}{v_{1a}} = \left(\frac{v_{1a}}{v_{1a}}\right)^{-1}
$$
\n
$$
T = \frac{v_{1a}}{v_{1a}}
$$

So

$$
Re_{l_o} = \frac{v_o l_o}{v}
$$

Damkohler number would be

$$
Da = \frac{\tau_o}{\tau_c} = \frac{l_o}{v_o} \frac{S_L}{\delta_L}
$$

Kolmogrov number is

$$
Ka = \frac{\tau_c}{\tau_\eta} = \frac{\nu_\eta}{\eta} \frac{S_L}{\delta_L} = \left(\frac{\delta_L}{\eta}\right)^2
$$

and turbulent intensity that would be TI which is

$$
TI = \frac{v_o}{S_L}
$$

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So, using these different number or non-dimensional numbers the one can define this diagram which is called the Borghi diagram. It defines the different ray this is a laminar flame then you can have wrinkled flamelets, so on this side you $\frac{l_t}{s}$ $\frac{l_t}{\delta_L}$ and on this side you go $\frac{u'}{u_L}$. This is a line which is Karlowitz number less than one corrugated flamelets in this is distributed reaction resume and this is oil start where the Damkohler number less than 1.

And this line corresponds to Damkohler number one and in this particular zone you have both Damkohler number and calories number gear up than 1.

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Then later on it was modified by Peters and it is a slightly I mean slight modification to that to see. So as I said this is a laminar zone this remains wrinkle flamelets. Then this region they say it is corrugated flamelets and this line corresponds to color is number 1. So this is a thin reaction

zone. And this is the so most of the flame front will lie in these zones and this is our broken reaction zone and all these, because once you have a piece of information about your geometry and your field and the competitions one can estimate where this flame is going to belong.

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Now, once you come to flamelet regimes, your Karlovitz number is getting that

$$
Ka = \frac{\tau_c}{\tau_\eta} = \frac{\nu_\eta}{\eta} \frac{S_L}{\delta_L} = \left(\frac{\delta_L}{\eta}\right)^2 < 1
$$

So that means if I plot a diagram for this is my let us say a flame front. This is the idea that is actually going to act on it. This is on the unburned side this is burned side. So the thickness of the reaction zone plus I can say this is reaction plus preheat zone the thickness of the reaction plus preheat zone is thinner than the Kolmogorov scale. So, which means it is $\delta_L < \eta$.

So, transport a mass on heat between the reaction zone and the preheat zone is bimolecular mixing and as a good approximation the local flame propagates at laminar speed and the thickness of the flame is laminar. So,

$$
\frac{\dot{m}_{kolm}}{\dot{m}_{rec,all\;lay}} \sim \frac{\frac{u(\eta)}{\delta_L}}{\frac{D}{\delta_L^2}} \sim \frac{\delta_L}{\eta} \frac{u(\eta)\eta}{D} \sim \frac{\delta_L}{\eta} < 1
$$

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Now, if we go to thin reaction zone there Karlowitz number is

$$
Ka = \frac{\tau_c}{\tau_\eta} = \left(\frac{\delta_L}{\eta}\right)^2
$$

So, Karlowitz number lies between 1 and 100. So, here the same thing if you look at it, you can see one zone here and one zone here, this is our unburned this is burned. So, it is our kind of tick that, here the reaction pockets will not pass the inner layer of the reaction zone. So here one can say that

$$
\frac{\dot{m}_{kolm}}{\dot{m}_{rec,all\;lay}} \sim \frac{\frac{u(\eta)}{\delta_L}}{\frac{\delta_L}{\delta_L^2}}
$$
\n
$$
\sim \frac{\frac{u(\eta)}{\delta_L}}{\frac{\eta}{\delta_L^2}}
$$
\n
$$
\sim \frac{\frac{\delta_L}{\eta}}{\frac{u(\eta)\eta}{D}}
$$

So different regime you see different kind of.

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If you go to the distributed reaction zone and you will hear Karlowitz number is essentially get 100 and the same flame front if I see then there will be unburned, burned and this would be a pocket where you can have a large what we says this will move so reactant pockets may pass the reaction zone without full conjunction. So in that case

$$
\frac{\dot{m}_{kolm}}{\dot{m}_{rec,all\;lay}} \sim \frac{\delta_L}{\eta} \frac{u(\eta)\eta}{D}
$$

$$
\sim \frac{\delta_L}{\eta}>1
$$

Or

$$
\frac{\dot{m}_{kolm}}{\dot{m}_{rec,all\;lay}} \sim \frac{\delta_{in}}{\eta} \sim 0.1 \frac{\delta_L}{\eta} \sim 0.1 K a^{1/2} > 1
$$

so, this is what happens in the reaction zone.

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Now this is TPF is the turbulent premixed flame. So, these propagate due to heat transfer to preheat zone to heat up the fuel-air above to cross over temperature and fuel-air mass transfer to the reaction zone to provide fuel-air. So, the transport of mass and heat between the reaction zone and preheat zone can be different for laminar premixed flames depending on the thickness of the zone.

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So, this is now, we have seen the flame speed. So, this is our fresh gas this is burnt gas, this is an iso-surface of the flame front. So,

$$
\frac{\partial c}{\partial t} + \overrightarrow{w} \, \overrightarrow{\nabla} c = 0
$$

c is the progress variable and c_f is iso level of the progress variable at maximum reaction rate so this is the convey equation an absolute speed would be \vec{w} . \vec{n} . So, this is how the velocity vector would be acting in this direction, this is u dt and this is w dt and S_d would be $(\vec{w} - \vec{u})\vec{n}$.

So, one is absolute speed, one is displacement speed and delta n is the unit normal vector which is calculated live ∇c by module of ∇c. So apart from that you can see now.

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If I start with this equation,

$$
\frac{\partial c}{\partial t} + \overrightarrow{w} \, \overrightarrow{\nabla} c = 0
$$

now use the union normal vector then I write this

$$
\frac{\partial c}{\partial t} + \overrightarrow{w} \cdot \overrightarrow{n} | \overrightarrow{\nabla} c | = 0
$$

and from here I can get absolute speed

$$
\vec{S}_a = \vec{w}.\vec{n} = \frac{1}{|\vec{\nabla}c|} \frac{\partial c}{\partial t}
$$

and then that will give me the displacement speed between these which is

$$
\vec{S}_d = \vec{w}.\vec{n} - \vec{u}.\vec{n} = \frac{1}{|\vec{\nabla}c|} \left(\frac{\partial}{\partial t} + \vec{u}\vec{\nabla}\right)c
$$

Now you can find these things, then we can find out the relationship between the displacement speed and the species equation using this information. So, we will stop here today and continue the discussion in the next lecture.