Fundamentals of Combustion

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Lecture - 27

Governing Equations for Reacting Flow – Part 4

Control of Combustion Phenomena and Simplified Chemically Reacting System

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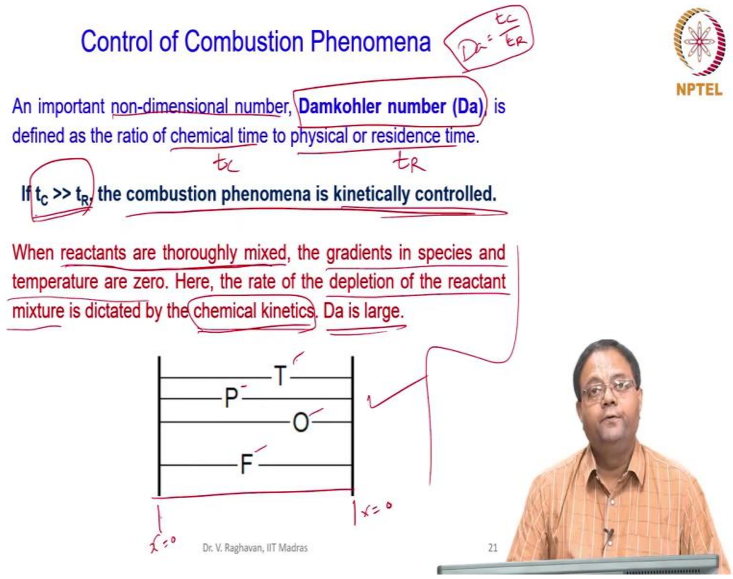

Control of Combustion Phenomena

$Da = \frac{t_c}{t_R}$

An important non-dimensional number, **Damkohler number (Da)** is defined as the ratio of chemical time to physical or residence time.

t_c t_R

If $t_C >> t_R$, the combustion phenomena is kinetically controlled.

When reactants are thoroughly mixed, the gradients in species and temperature are zero. Here, the rate of the depletion of the reactant mixture is dictated by the chemical kinetics. Da is large.

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So, the important non dimensional number called Damkohler number, that is defined as a ratio of chemical time t_C and the physical or residence time t_R. So, Damkohler number is very important number which is defined as t_C/t_R.

So, based upon the Damkohler number, we can say the category of the control of the combustion phenomena. When t_C, the chemical time, is much higher than the flow residence time t_R, then the combustion phenomena is kinetically controlled.

So, what happens here, reactants are thoroughly mixed. For example, this is the chamber in which I am having some reactants. So, fuel and oxidizer, on the completion of the reaction products will be formed and it has some temperature.

So, temperature when the reactants are present in this chamber it will be T_u and when the products are formed it will be T_F. So, let us say this is the scenario, but at every time instant everything is well mixed here. So, thoroughly mixed. This is say $x = 0$ to $x = l$, there is no gradient, there is a well-mixed or uniformly distributed reactants are present.

Now, after the completion of combustion, products will be uniformly present in this. So, the gradients of species and temperature are negligible, zero. So, in this case when the reactants are present and you ignite it, the depletion or the reactant consumption will depend only on the chemical kinetics, based upon the temperature.

This is totally controlled by the kinetics, the phenomena of combustion here. The Damkohler number is very large. Because you can see t_C/t_R, t_R is very small and tends to 0. So, Damkohler tends to infinity.

So, Damkohler number is very large. This is the regime where $t_R << t_C$, it will take some finite time for the reaction to complete. That is the phenomena is kinetically controlled. So, for analyzing this, it may be ignition, I take a small volume where there is a well mixed reactant.

So, I try to put some energy to ignite it. From the initial temperature it goes to a higher temperature. So, that ignition process is kinetically controlled. So, that is the first category in which you will understand that there is no other gradient. So, I am actually having no gradient in the fuel, oxidizer or temperature and so on. Only the kinetic is going to help us solving this problem.

So, how much time it will take for temperature to rise from the initial value to the final value, that will be only dependent on the chemical kinetics. So, that is the first category in which the transport processes are not at all present. The residence time is very negligible, finite rate of kinetics is required. That means, it will take some time for the reaction to complete. So, that is what the first category is.

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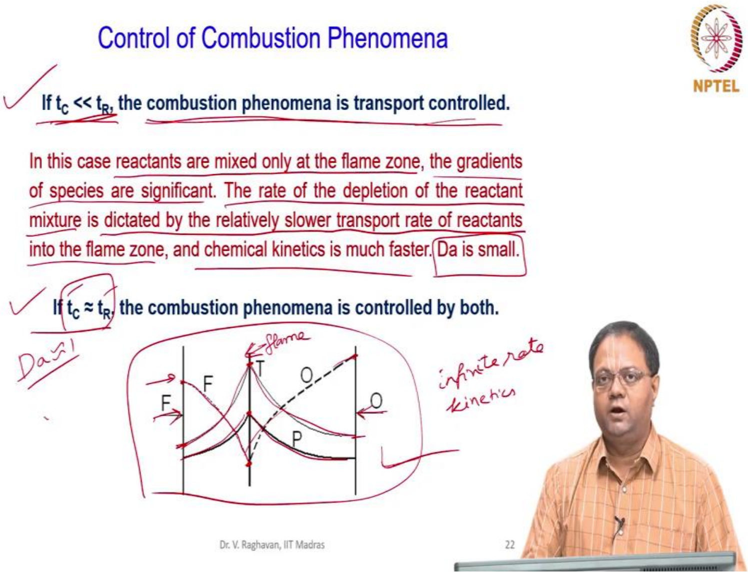

Control of Combustion Phenomena

If $t_C << t_R$, the combustion phenomena is transport controlled.

In this case reactants are mixed only at the flame zone, the gradients of species are significant. The rate of the depletion of the reactant mixture is dictated by the relatively slower transport rate of reactants into the flame zone, and chemical kinetics is much faster. Da is small.

If $t_C \approx t_R$, the combustion phenomena is controlled by both.

The second category t_C chemical time is much much lesser than the t_R, the residence time, then the combustion phenomena is transport controlled.

Now, this is the figure, fuel is supplied from one side and oxidizer is supplied from another side, you can see that fuel is higher here where it is supplied, similarly oxidizer is higher here from where it is supplied. Slowly fuel and oxidizer is consumed. When they are consumed completely you get the flame zone. So, this is the flame zone actually. So, this is the non-premixed flame the other extreme category, in the previous category everything was very well mixed, the fuel and oxidizer and uniform temperature it was in. But, here you can see that the fuel can have a different temperature and oxygen can have a different temperature, they come in and mix. Once they mix, instantaneously chemical reaction will take place that is the meaning of this.

So, when they diffuse and mix at a particular point at stoichiometric proportion, they just react very fast like this flame here. It has a chemical time which is negligible. The reaction rates are much higher than when compared to the time it requires for the transport these reactants towards the flame.

So, you can see the gradient of the fuel here. Strong gradient of fuel or oxidizer is present. Similarly, temperature which is reaching maximum at the flame zone can have a gradient towards these streams like this. Similarly, products which are formed at the flame zone will diffuse towards the fuel side and towards the oxidizer side and so on.

So, clearly you can see that there are gradients as opposed to a 0 gradient scenario for the kinetically controlled combustion. Here, chemical time is negligible. As and when the fuel and oxidizer are meeting at stoichiometric proportion instantaneously they react. So, this is also called infinite rate chemistry.

So, infinite rate kinetics. The chemical kinetics is so fast, then it can be assumed to be occurring at an infinitely faster rate. The reaction is going to finish within some negligible time, but the fuel and oxidizer are transported towards that point that will take more time. So, that is going to control the phenomena that is the second phenomena here, reactants are mixed only at the flame zone, they are not premixed.

The gradients of the species are significant as indicated here, the rate of depletion of the reactant mixture is dictated by the relatively slower transport rate of reactants towards the flame zone, chemical kinetics is much faster. Damkohler number tends to 0. The previous case, Damkohler number was very large. Here, Damkohler number goes 0.

The third category is the category, where both the times are of same order t_C chemical time, t_R residence time are of same order, then you cannot neglect anything both are important. That is the third phenomena. So, here $t_C >> t_R$. Damkohler number is very large and a fully kinetically controlled regime exists.

Second extreme is $t_C << t_R$, you can see the gradients, chemical kinetics is very fast. The transport is going to control, when I say infinitely fast chemistry, I do not need kinetics at all to analyze this flame.

You do not need to worry about single step, multi-step, elementary and global reactions, nothing is required. Only the rate at which the fuel and oxidizer are going to be fed here that will dictate the formation of flame. See for example, if we take this scenario, if I now increase the fuel flow rate the flame will shift to the right. Or if I increase the oxygen flow rate the flame will shift to the left.

So, that is the way we see this. When I increase the fuel flow rate, fuel requires more oxygen, the oxygen is fed at the same rate. So, the fuel will now go towards oxygen side the flame will shift towards that.

So that means by controlling the flow rates, I can locate the flame anywhere I want. See if the momentum of these two jets are kept constant, then I can see that this flame can be at center.

So, I can adjust my flame location based upon the control of flow rates, that is transport controlled. I do not need to worry about the kinetics, kinetics is very fast already, whenever they mix they will react. So, that is the tendency of the chemical kinetics there. So, that is second extreme.

The third is you have to care for both, where you have Damkohler number approaching 1, you have to care for both. So, in the flame you have to incorporate some kinetics to analyze the problem and again you have to resolve the flow process also properly.

So, both have to be done in this third category. First category I do not really worry about the flow process or any diffusion, I only worry about the kinetics here. Second I do not worry about kinetics at all I only worry about the flow, how to properly resolve the flow, the third I have to worry about both, I will take care of both.

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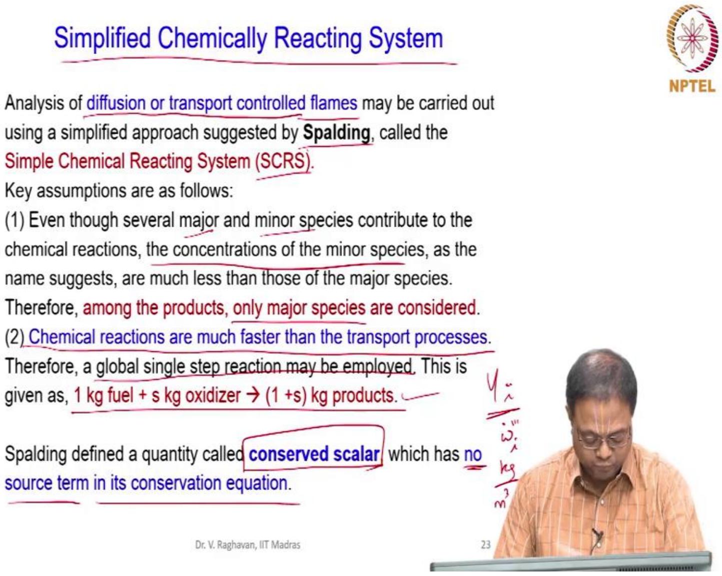

Simplified Chemically Reacting System

Analysis of diffusion or transport controlled flames may be carried out using a simplified approach suggested by **Spalding**, called the Simple Chemical Reacting System (SCRS).

Key assumptions are as follows:

(1) Even though several major and minor species contribute to the chemical reactions, the concentrations of the minor species, as the name suggests, are much less than those of the major species. Therefore, among the products, only major species are considered.

(2) Chemical reactions are much faster than the transport processes. Therefore, a global single step reaction may be employed. This is given as, 1 kg fuel + s kg oxidizer → (1 +s) kg products.

Spalding defined a quantity called **conserved scalar** which has no source term in its conservation equation.

Y_i

$\dot{\omega}_i'''$

$\frac{kg}{m^3}$

Now, we have seen the governing equation which are actually pretty complicated equation. You can see that for example, for reactive flows the set of species conservation what you are going to get. Those species conservation equation, if there are N species capital N species, we will have to solve N-1 partial differential equations and these equations will have a non-linear source term.

So; that means its really complicated to solve this when you have a non-linear source term, which is exponentially dependent on temperature. A slight increase or decrease in temperature will affect the source term and affect the solution of this.

You have to solve it numerically and this numerical solution will suffer when there is abrupt change. So, we have to really worry about imparting changes at a smaller level and merge the solution especially if it is time dependent and so on.

On the other hand, if you see the energy equation, you have fluxes due to diffusion of species enthalpy. Similarly, you have the source term $\dot{\omega}'''$ h_i. So, these terms are non-linear source terms which we have.

So, what happens here, again the solution is complicated. So, is there any way we can simplify this. See the category 2 here and to some level to category 3, we can try to minimize the chemical kinetics. So, mainly due to the chemical kinetics the non-linear terms are arriving. So, if you have scenario where diffusion or transport phenomena or processes are going to control the flames, then we can go for what is called simplified chemically reacting system, which was introduced by Professor Spalding. Simple or simplified chemical reacting system SCRS. There are some assumptions made in this system. So, we have major products, minor products etcetera. So, all we have seen the elementary reactions with lot of radicals like O, H, HO, H_2O etcetera HO_2 lot of things are there.

So, major products are CO_2 and H_2O. The concentrations of the minor species O, H, OH and this HO_2 etcetera are very less. So, we will not worry about the minor species. We will only consider the major species. Second is chemical reactions are going to be very fast and transport process are very slow.

So, in that case I do not need to worry about multi step reactions. I go only for a single step reaction and this is given like this. 1 kg of fuel + s kg of oxidizer → 1 + s kg of products. This is the reaction I consider. So, these are the assumptions made and Spalding defined a quantity called conserved scalar. See for example, mass fractions is a scalar, but it has a non-linear source term.

For example, when you consider Y_i you have a non-linear source term $\dot{\omega}_i'''$. So, this is kg/m^{3}s. So, that source term arrives. But, if you have a scalar which is called conserved scalar, then there will be no source term in the conservation equation, how will you define such variable that is what we have to see.

So, my main intention of this simple chemical reaction system is to eliminate the source terms, because, I do not want chemical kinetics. The interaction of chemical kinetics is very minimum or negligible here. So, how can we eliminate the chemical kinetics and concentrate on the transport processes that is what we are trying to see here.

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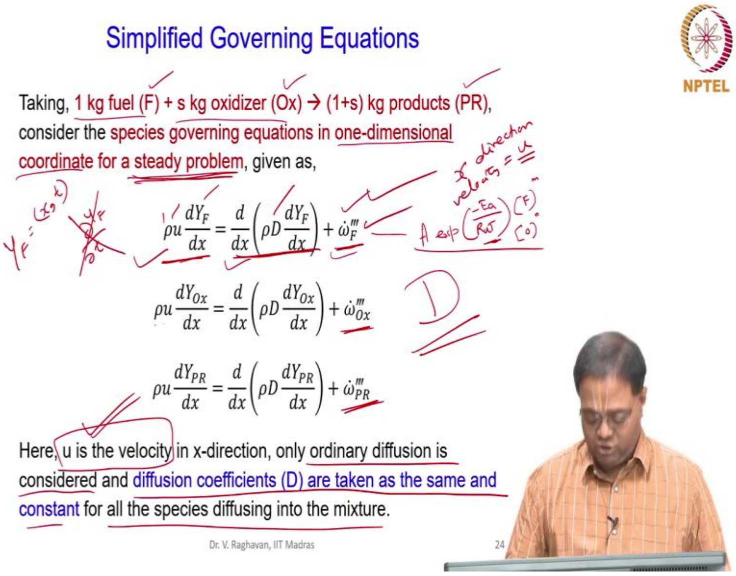

Simplified Governing Equations

Taking, 1 kg fuel (F) + s kg oxidizer (Ox) → (1+s) kg products (PR), consider the species governing equations in one-dimensional coordinate for a steady problem, given as,

$$\rho u \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}_F'''$$

$$\rho u \frac{dY_{Ox}}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_{Ox}}{dx}\right) + \dot{\omega}_{Ox}'''$$

$$\rho u \frac{dY_{PR}}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_{PR}}{dx}\right) + \dot{\omega}_{PR}'''$$

Here, u is the velocity in x-direction, only ordinary diffusion is considered and diffusion coefficients (D) are taken as the same and constant for all the species diffusing into the mixture.

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$Y_F = (x, t)$

x direction velocity = u

$A \exp\left(\frac{-E_a}{R_u T}\right) [F]^m [O]^n$

D

So, taking the same global reaction 1 kg of fuel and s kg of oxidizer so, I am saying fuel is F oxidizer is Ox and products is PR, I am not taking into account of products like H_2O,

CO_2 etcetera just group everything and call it product stream PR. Now, let us consider for simplicity one dimensional coordinate say x coordinate.

And we also consider steady problem. Transient term $\partial u / \partial t$ is neglected. So, I get ordinary differential equation rather than the partial differential equation.

So, when I write the conservation for fuel what I get is convective term. So, x direction velocity is u. So, u is the x direction velocity and ρ is the mixture density, I am considering mass fraction of the fuel. So, dY_F/dx, there is no transient term. If I put a transient term, then Y_F will be a function of x and t. So, ordinary differential equation will be converted into a partial differential equation. I will add this term.

So, this is a steady problem. So, I write an ordinary differential equation here. So, this plus I am just considering ordinary diffusion. Please understand I do not consider this any complicated diffusion, Soret effect etcetera here. So, ordinary diffusion I have a diffusion coefficient. So, this is the diffusion term. So, convection of the species, this is diffusion of the species and the source term. Source term has not been eliminated so far.

So, the source term remains, that means, obviously, the scalar Y_F is not conserved scalar it has a non-linear source term. So, this is the way I write the convective term, the diffusion term and source term.

$$\rho u \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}_F'''$$

Write same thing for the oxidizer

$$\rho u \frac{dY_{Ox}}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_{Ox}}{dx}\right) + \dot{\omega}_{Ox}'''$$

Then products,

$$\rho u \frac{dY_{PR}}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_{PR}}{dx}\right) + \dot{\omega}_{PR}'''$$

So, these three equations you can see that there are non-linear source terms, one more assumption what I make is I know u. If I want to solve for u I have to again solve for continuity equation, the mass conservation of the mixture and the momentum equation together, if I solve then I will get the u.

Let us assume that u is known to us now. Or its not a problem to solve u also by solving the momentum equation along with continuity, I can solve for u and its one dimensional. It is simplified now please understand that as I told before I am considering only the ordinary diffusion, Soret diffusion is also neglected that is fine for us.

Then one more assumption what I have made here is the diffusion coefficient D are taken as the same, for all this, fuel, oxidizer or products the diffusion coefficient D is same that is what the third thing I am using here. So, I am simplifying, as I told you I need not calculate this, when we discussed about the thermal physical properties here.

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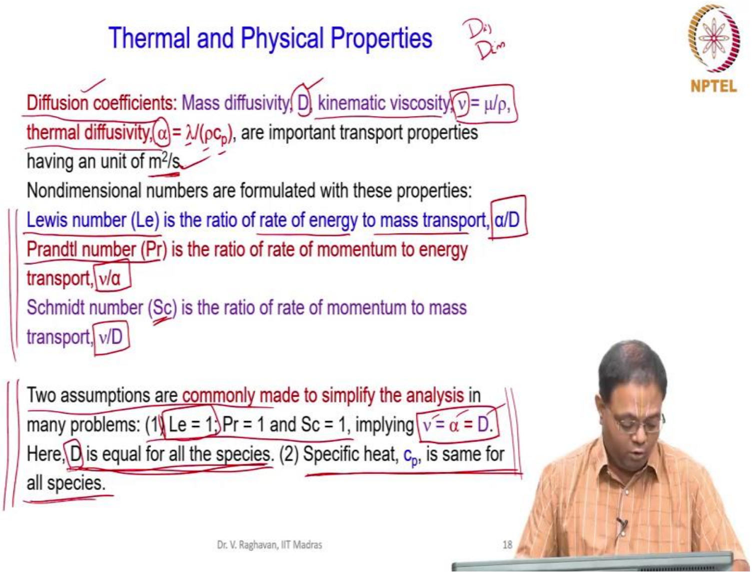

Thermal and Physical Properties

D_i
D_{im}

Diffusion coefficients: Mass diffusivity, $\boxed{D}$, kinematic viscosity, $\boxed{\nu = \mu/\rho}$, thermal diffusivity, $\boxed{\alpha} = \lambda/(\rho c_p)$, are important transport properties having an unit of m^2/s.

Nondimensional numbers are formulated with these properties:

Lewis number (Le) is the ratio of rate of energy to mass transport, $\boxed{\alpha/D}$

Prandtl number (Pr) is the ratio of rate of momentum to energy transport, $\boxed{\nu/\alpha}$

Schmidt number (Sc) is the ratio of rate of momentum to mass transport, $\boxed{\nu/D}$

Two assumptions are commonly made to simplify the analysis in many problems: (1) $\boxed{Le = 1}$; Pr = 1 and Sc = 1, implying $\boxed{\nu = \alpha = D}$. Here, $\boxed{D}$ is equal for all the species. (2) Specific heat, c_p, is same for all species.

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We already told that I can say D is equal for all the species. Two assumptions which commonly made are this, Lewis number is equal to 1. I will also take the D the diffusion coefficient for particular species going to the mixture to be same for all the species.

Similarly, I can also invoke this specific heat is same for all the species, these are the simplified assumptions I invoke. Because, if you see for a mixture, there is no big change, again it may be a dependent on temperature or not that is second question.

If it is not dependent on temperature, then we have to calculate this at a particular temperature called average temperature, we will come to that in the later part. What I am assuming here is instead of using individual values for D of a particular species going into a mixture; I am assuming that the D is same for all the species that is one of the important assumptions.

So, with that assumption here you see that the diffusion coefficients are taken as the same so, that will give you this. So, ρD here is same for all the species F, Ox and PR. This is one dimensional, still we have not eliminated the non-linear terms, solving this is again not easy.

Because of the non-linearity in the source term, you can see this will depend on say A $\exp(-E_a/R_uT)[F]^m\ O]^n$, this will be the equation here. So, you can see the exponential dependence on this temperature here.

So, any small variation in temperature will cause a huge difference in this value. That may make the numerical scheme to oscillate, some instability can occur. So, how to avoid that. That means that we have to very carefully proceed with the solution of this equation. When there is an exponential dependence on temperature for the source terms.

So, elimination and we do not require this, that is a main criteria here. For diffusion controlled or transport controlled flames we can eliminate this. So, how we will do this that is the question. Now, we will say that u is known to me or by solving the continuity and momentum equation, we can take u we will not worry about u much.

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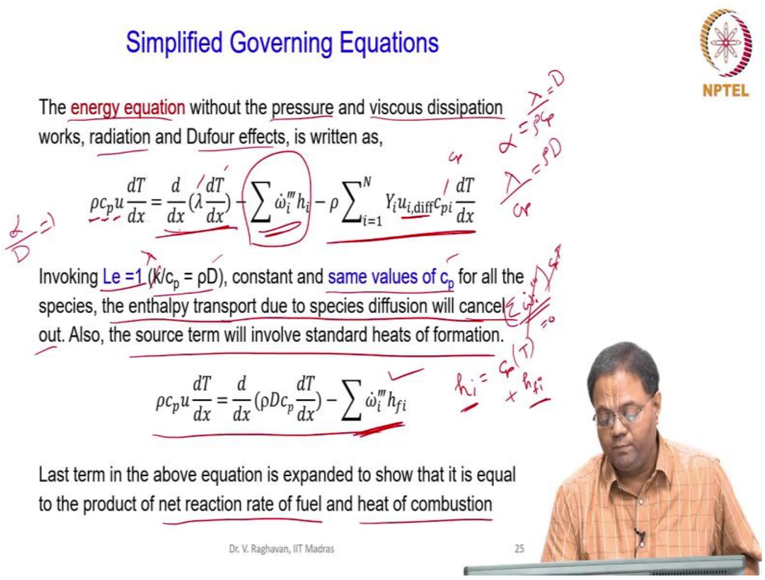

Simplified Governing Equations

The energy equation without the pressure and viscous dissipation works, radiation and Dufour effects, is written as,

$$\rho c_p u \frac{dT}{dx} = \frac{d}{dx}(\lambda \frac{dT}{dx}) - \sum \dot{\omega}_i''' h_i - \rho \sum_{i=1}^{N} Y_i u_{i,\text{diff}} c_{pi} \frac{dT}{dx}$$

Invoking Le =1 (k/c$_p$ = ρD), constant and same values of c$_p$ for all the species, the enthalpy transport due to species diffusion will cancel out. Also, the source term will involve standard heats of formation.

$$\rho c_p u \frac{dT}{dx} = \frac{d}{dx}(\rho D c_p \frac{dT}{dx}) - \sum \dot{\omega}_i''' h_{fi}$$

Last term in the above equation is expanded to show that it is equal to the product of net reaction rate of fuel and heat of combustion

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$\frac{\lambda}{\rho c_p} = D$

$\alpha = \frac{\lambda}{\rho c_p}$

$\frac{\lambda}{c_p} = \rho D$

$\frac{\alpha}{D} = 1$

$h_i = c_p(T) + h_{fi}$

Now, energy conservation, again I am writing this without the pressure, viscous dissipation work terms, radiation also neglected. Dufour effect as usual is neglected and one dimensional transient term is neglected. So, one dimensional only, the ordinary derivative is written here, $\rho c_p u(dT/dx) = d/dx(\lambda dT/dx)$, the conduction term.

$$\rho c_p u \frac{dT}{dx} = \frac{d}{dx}(\lambda \frac{dT}{dx}) - \sum \dot{\omega}_i''' h_i$$
$$- \rho \sum_{i=1}^{N} Y_i u_{i,\text{diff}} c_{pi} \frac{dT}{dx}$$

Then, again you can see the non-linear terms are there $\dot{\omega}_i'''$ h_i summed over all the species and you can see the diffusional flux of each species due to the temperature gradient here, $\rho Y_i u_{i,\text{diff}}$ is the diffusional flux into the enthalpy. So, that diffusion to the surfaces.

Now, here I invoke Lewis number equal to 1, I already shown that these non-dimensional numbers can be same. So, when we say Lewis number equal to 1, $\alpha/D = 1$. What is α? $\alpha = \lambda/\rho c_p = D$.

So that means, lambda by c_p equal to rho into D. So, that is what I have written here. This is actually $\lambda/c_p = \rho D$. So, thermal conductivity, k or λ represent thermal conductivity.

I am also taking the second assumption same values for the c_p's of all the species. That also I am invoking here. So, the diffusion coefficient of all the species are same. Similarly, the c_p's of each species is same.

So, by invoking this I can simplify this equation further. Now, what else I am doing here, when i say c_{pi} is just c_p, c_{pi} of all the species are same, there is only c_p. Now, what happens? Then this $c_p dT/dx$ will be constant that can be taken out and then what I have is only $\rho_i u_{i,diff}$, that will be the diffusion flux.

So, diffusion flux summed over multiplied by $c_p dT/dx$ that will cancel out this term. Then the source term, I can write this as, $h_i = c_p T + h_{fi}$.

So, now if I say $c_p T$ and when I sum it over all this, so, this can be written in this term h_{fi} only will come into play, because $c_p T\ \dot{\omega}_i'''$, we can write this term.

So, when I substitute here you will write $\sum \dot{\omega}_i'''\ c_p T$. So, this will be equal to 0 when I add the source term of all the species some will be produced some will be destroyed. So, that the net rate of production will be equal to net rate of consumption.

So, $\sum \dot{\omega}_i'''$ over all the species will be equal to 0. So, this term will be written only in terms of heat of formation. So, $\sum \dot{\omega}_i'''\ h_{fi}$, still this source is there. So, now, you can see that there is a source term which is non-linear in nature ok again you can see.

So, this particular term can be further expanded. The last term of the above equation is expanded, now further to show that it is equal to the product of net reaction rate of fuel and the heat of combustion.