Combustion in Air Breathing Aero Engines
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Lecture – 16
Governing Equations IV

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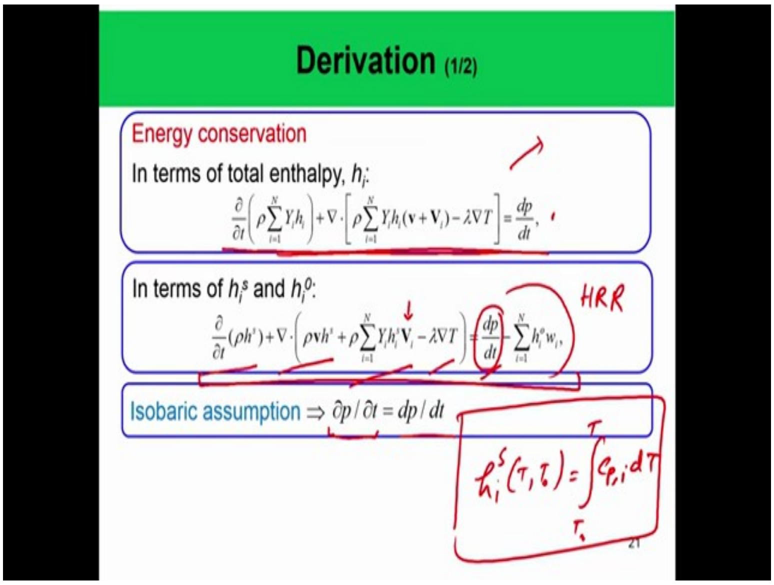

Derivation (1/2)

Energy conservation

In terms of total enthalpy, h_i:

$$\frac{\partial}{\partial t}\left(\rho\sum_{i=1}^{N}Y_ih_i\right)+\nabla\cdot\left[\rho\sum_{i=1}^{N}Y_ih_i(\mathbf{v}+\mathbf{V}_i)-\lambda\nabla T\right]=\frac{dp}{dt},$$

In terms of h_i^s and h_i^0:

$$\frac{\partial}{\partial t}(\rho h^s)+\nabla\cdot\left(\rho\mathbf{v}h^s+\rho\sum_{i=1}^{N}Y_ih_i^s\mathbf{V}_i-\lambda\nabla T\right)=\frac{dp}{dt}-\sum_{i=1}^{N}h_i^o w_i,$$

HRR

Isobaric assumption $\Rightarrow \partial p/\partial t = dp/dt$

$$h_i^s(T,T_0)=\int_{T_0}^{T}c_{p,i}\,dT$$

So, now what we have got is with; this is our final clinked of on that you get, that is the in terms of the total this is what we have essentially done. We had from the; this is the internal energy equation; we have obtained this equation for total enthalpy and then we have obtained in terms of the species; in terms of the sensible enthalpy; how? We just took this total enthalpy equation and then we took the equation for the species mass fraction. We multiplied the species mass fraction equation with the corresponding enthalpy of formation for i-th species and then be subtracted that in some (Refer Time: 01:03) for i is equal to 1 to N and then we subtracted that equation from this equation and then we are left with essentially is the equation for the sensible enthalpy.

So, this is once again we have seen; that this is a transient term and this is a convection term and this is the term that we get because of different heat capacities and that because of because species of different heat capacities are crossing the boundary or crossing the control surface or the element surface, infinite decimal control volume surface; through U with this species diffusion velocity and of course, energy is crossing the control surface through lambda delta T and then there is a there should dp; dt term and this is the very important heat release rate term, which we will be denote by HRR. So, this is the question that we have got and then of course, you can ask that why have we used dp; dt because of the isobaric assumption.

We our pressure does not depend on special locations or it does not depends on in space; it does not change in space; we are in let us constant and hence dou P dou T is especially dp; dt is a p is only a function of temperature and from that as we know that because h i S; T with respect to T 0 is nothing but integral T 0 to T 0 to T C P; i dT because of this equation because of the h; dt essentially C P; i that is the definition of C P; i. We can convert this equation into a equation of temperature and that is a very common form this is how we actually solve the energy equation in a CFD code or when you are analytically computing some flames.

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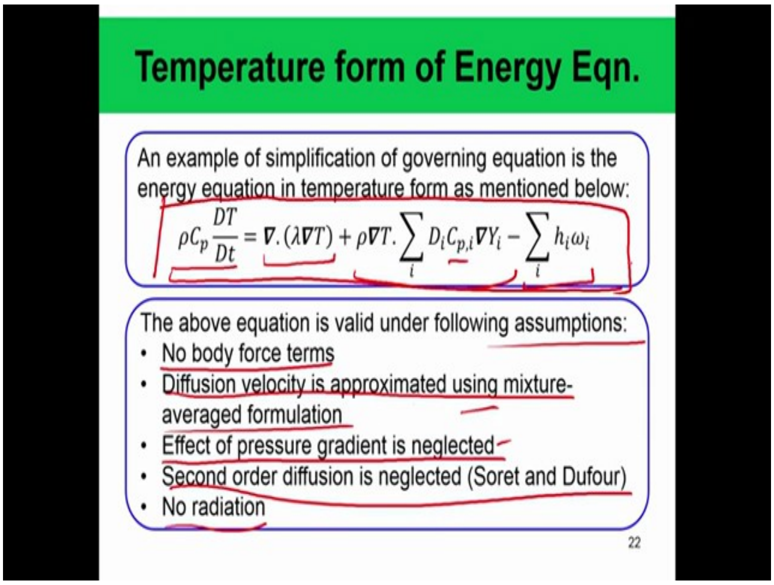

Temperature form of Energy Eqn.

An example of simplification of governing equation is the energy equation in temperature form as mentioned below:

$$\rho C_p \frac{DT}{Dt} = \nabla.(\lambda \nabla T) + \rho \nabla T. \sum_i D_i C_{p,i} \nabla Y_i - \sum_i h_i \omega_i$$

The above equation is valid under following assumptions:

- No body force terms
- Diffusion velocity is approximated using mixture-averaged formulation
- Effect of pressure gradient is neglected
- Second order diffusion is neglected (Soret and Dufour)
- No radiation

And this is the example of simplification; it involves a more simplification also are with some assumptions also I will come later so, but this is equation that is rho C P; that is total derivative of temperature essentially this diffusion term, there is a heat conduction term minus the plus of course, this one that is which arises due to the difference C P i's and that then the heat (Refer Time: 03:26).

Now, then the equation is these equation is valid under of course, following assumptions you must remember, but this is the equation that you have to solve in addition to other equations; if you have to if you are solving for combustion in a CFD code for analytical calculation as I said but this equation is valid only under this could following conditions and these are that we do not use any body force term and the diffusion velocity is approximated using a mixture averaged formulation.

I will come to that later that is and then we have that is similar to this D i N; essentially, but we assumed that it is this diffusing species is diffusing in a bulk have that mixture other than in a particular species. Then we have neglected the effect of pressure gradient and second order diffusion in terms of Soret and Dufour neglected and there is no radiation. So, these are the restricted assumptions, so if this secretion; if this assumptions are suitable for your condition, you can use this equation in our CFD calculation or a analytical calculation.

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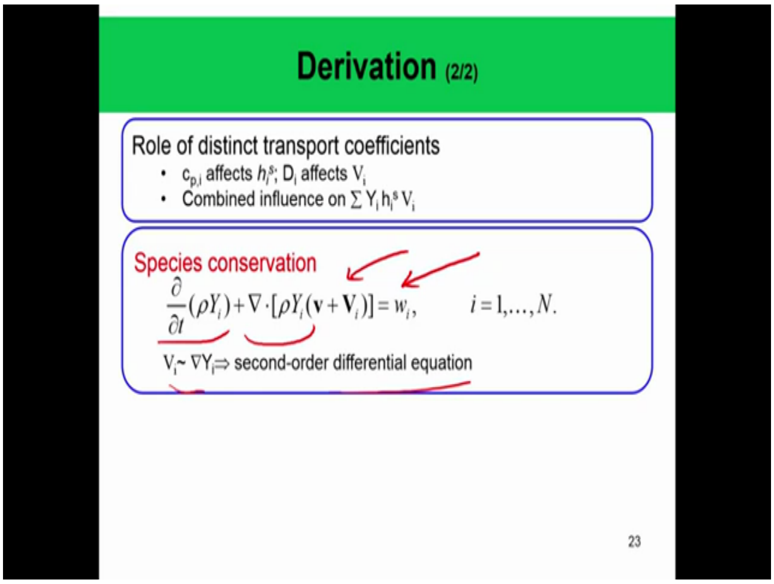

Derivation (2/2)

Role of distinct transport coefficients

- $c_{p,i}$ affects h_i^s; D_i affects V_i
- Combined influence on $\sum Y_i h_i^s V_i$

Species conservation

$$\underbrace{\frac{\partial}{\partial t}(\rho Y_i)}+\nabla\cdot[\underbrace{\rho Y_i}(\mathbf{v}+\mathbf{V}_i)]=w_i, \qquad i=1,\ldots,N.$$

$V_i \sim \nabla Y_i \Rightarrow$ second-order differential equation

So, now we need to basically see as we have seen that this is the species concentration. So, this is of course the species equation then that this transient term. Once again and this is the confection term and this term arises once again because of the species can cross the control surface with different species diffusion velocities and of course, this is the species production rate term; in terms of elements of mass. We have of course, used this is this we have assumed that V i is essential proportional to gradient of the species mass fraction.

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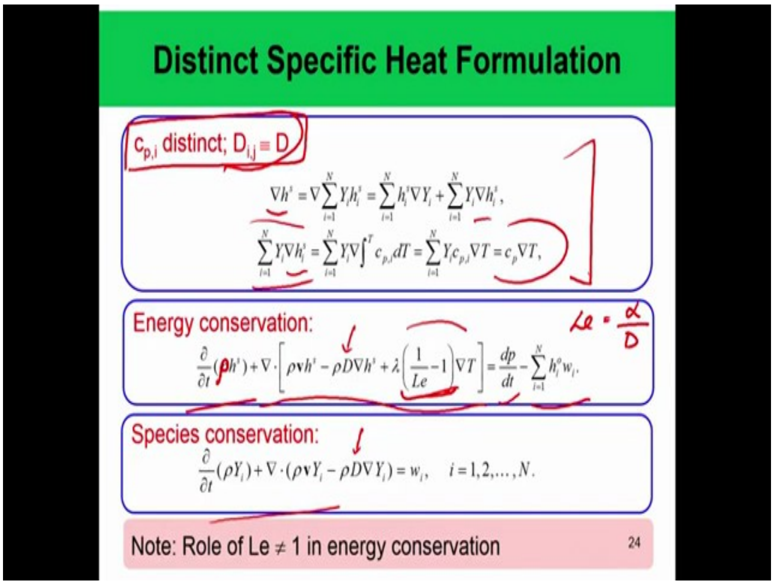

Distinct Specific Heat Formulation

$c_{p,i}$ distinct; $D_{i,j} \equiv D$

$$\nabla h^s = \nabla \sum_{i=1}^{N} Y_i h_i^s = \sum_{i=1}^{N} h_i^s \nabla Y_i + \sum_{i=1}^{N} Y_i \nabla h_i^s,$$

$$\sum_{i=1}^{N} Y_i \nabla h_i^s = \sum_{i=1}^{N} Y_i \nabla \int^{T} c_{p,i} dT = \sum_{i=1}^{N} Y_i c_{p,i} \nabla T = c_p \nabla T,$$

Energy conservation:

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

$$\frac{\partial}{\partial t}(\rho h^s) + \nabla \cdot \left[\rho \mathbf{v} h^s - \rho D \nabla h^s + \lambda \left(\frac{1}{Le} - 1 \right) \nabla T \right] = \frac{dp}{dt} - \sum_{i=1}^{N} h_i^o w_i.$$

Species conservation:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \mathbf{v} Y_i - \rho D \nabla Y_i) = w_i, \quad i = 1, 2, \ldots, N.$$

Note: Role of Le ≠ 1 in energy conservation

Now, we can simplify this as you see that this all the C p i j or D i j; these are difficult to handle. So, we will consider two limits; the first limit is that we will consider that the C P; i that the specific heat is species specific, but our D i j is equal to constant is equal to d. So, then we can see that this we can write this gradient of enthalpy in this form and we will see that we can write this guy this summation of i is equals to 1 to N; Y i times a gradient of h i s; in essentially as a c p times gradient of T.

And anyways, the final equation that we get; you can all ready also do this derivation and what we finally, get is that under this restriction that our C P; i is distinct, but our diffusivity are constant which is equal to D and we are get this equation this is essentially density and we will see that this is the equation that is get is d rho d i h s; dt is plus which is the thing divergence of rho v h s minus rho D gradient of h s.

Here we see a Lewis number coming Lewis number is nothing but thermal diffusivity by the species diffusivity. So, this is thing that we get now here we get a Lewis number dependent and then you of course, have a pressure derivative dp; dt minus the heat restrictor. And this is the species conservation that we get of course, the pointer not here is that and both to note here is that this D is essentially constant; so which is not affected the fact that we have assumed distinct specific heats, but constant diffusivities and D similar diffusivities are this D i j is equal to D.

So, now interesting point is to note that this Lewis number is comes up in the energy equation and which clearly tells that; if the Lewis number is not equal to 1; that if this say for example, Lewis number is greater than 1; this term will be negative and it will essentially act in some other way, whereas Lewis number is if it is less than 1, then this term will be positive and it will act in a different way.

Then the Lewis number is essentially can act as a source or sink in this energy equation; this Lewis number dependent times gradient of T. So, this is one interesting observation that Lewis number first shows up in a natural governing equations, when you do the distinct specific heat formulation.

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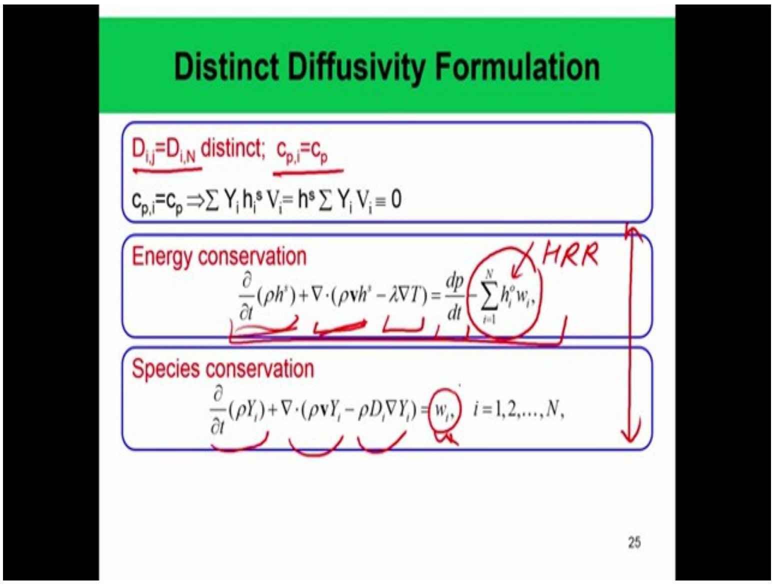

Distinct Diffusivity Formulation

$D_{i,j}=D_{i,N}$ distinct; $c_{p,i}=c_p$

$c_{p,i}=c_p \Rightarrow \sum Y_i h_i^s V_i = h^s \sum Y_i V_i \equiv 0$

Energy conservation

$$\frac{\partial}{\partial t}(\rho h^s)+\nabla\cdot(\rho \mathbf{v} h^s-\lambda\nabla T)=\frac{dp}{dt}-\sum_{i=1}^{N} h_i^o w_i,$$

HRR

Species conservation

$$\frac{\partial}{\partial t}(\rho Y_i)+\nabla\cdot(\rho \mathbf{v} Y_i-\rho D_i\nabla Y_i)=w_i, \quad i=1,2,\ldots,N,$$

So, but if you do the distinct diffusivity formulation; that is you assume the this specific heat are essentially same and D i j is equal to D i N and then you get you do not have the term because now your constant specific heat, as we discussed; the second term summation over Y i; h i; V i- capital V i that term drops out and you get a simplified energy conservation equation which is nothing but this d rho dt, d rho; h s dt plus this confection of enthalpy. So, the enthalpy can be changed by when rho h s that is the enthalpy itself is a is a function of time and then you have this enthalpy is confected and then you have heat conduction coming from a temperature gradient and then you have pressure derivative and then you have a heat release.

Once again this is the heat release rate term and then you have of course, the species conservation, so now you see that this is actually very useful form; which often people use, because there is an constant specific heats and diffusivities are different and here we the species conservation we see once again that this is the transient term and then this is a confection term, this is the species diffusing term and this is the species production or consumption rate that all depending on the sign.

Basically, if you see the chemistry is comes into here and into here and through; so, what will happens is that; you see these two another interesting thing to notice that this energy equation and the species equation at this form it is interesting to note that these two are coupled, how it is coupled? That can you see it is not apparent because this essentially h S is become writes in terms of temperature also; it is coupled actually, so, they have with these things.

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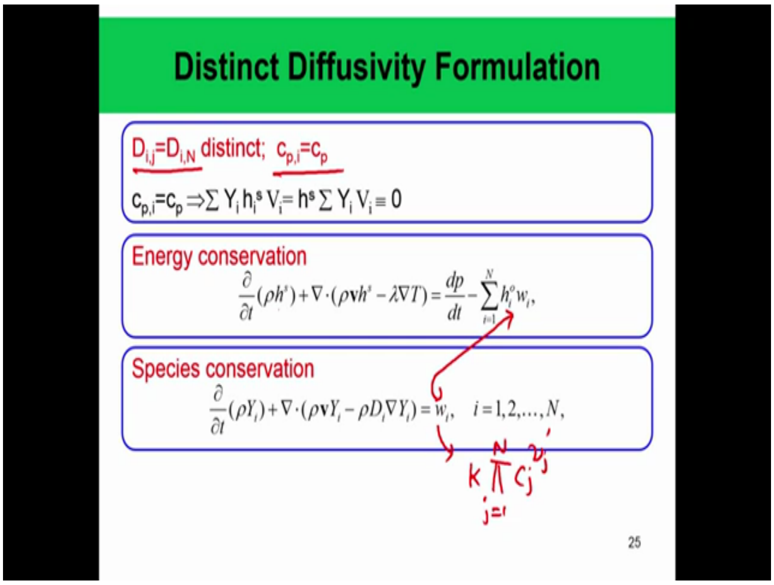

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$c_{p,i}=c_p \Rightarrow \sum Y_i h_i^s V_i = h^s \sum Y_i V_i \equiv 0$

Energy conservation

$$\frac{\partial}{\partial t}(\rho h^s)+\nabla\cdot(\rho \mathbf{v} h^s-\lambda\nabla T)=\frac{dp}{dt}-\sum_{i=1}^{N} h_i^o w_i,$$

Species conservation

$$\frac{\partial}{\partial t}(\rho Y_i)+\nabla\cdot(\rho \mathbf{v} Y_i-\rho D_i\nabla Y_i)=w_i, \quad i=1,2,\ldots,N,$$

$$K\prod_{j=1}^{N} C_j^{\nu_j'}$$

So, this omega i if you remember this as a form of like K times production that have C j; nu j dashed, j is equal to 1, 2; j is equals to 1 to N and of course, this also comes here and let us write it down.

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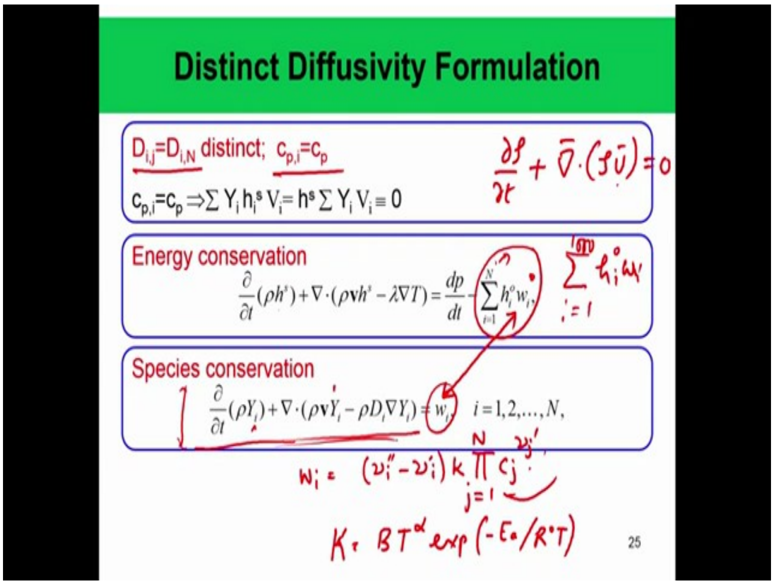

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$c_{p,i}=c_p \Rightarrow \sum Y_i h_i^s V_i = h^s \sum Y_i V_i \equiv 0$

$$\frac{\partial \rho}{\partial t} + \bar{\nabla}\cdot(\rho \bar{v}) = 0$$

Energy conservation

$$\frac{\partial}{\partial t}(\rho h^s) + \nabla\cdot(\rho \mathbf{v} h^s - \lambda \nabla T) = \frac{dp}{dt} - \sum_{i=1}^{N} h_i^o w_i, \qquad \sum_{i=1}^{N} h_i^o w_i$$

Species conservation

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla\cdot(\rho \mathbf{v} Y_i - \rho D_i \nabla Y_i) = w_i \quad i = 1,2,\ldots,N,$$

$$w_i = (\nu_i'' - \nu_i') k \prod_{j=1}^{N} c_j^{\nu_j'}$$

$$K = B T^{\alpha} \exp(-E_a/R^o T)$$

So, to this see basically how this coupling happens; so what I say is that its. This coupling between this two things happened to here and the coupling happens because omega i is nothing but nu i double dashed minus nu i dashed if you assume a one step reaction that omega i is essentially contribute from one reaction itself of course, it is coming from all reactions and we have to sum over all k, but I will not go to that right now and then you have the k term that is a this k is reaction rate constant times the continued product j is equal to 1 to c j times nu j dashed and then k is nothing but B times T to the power of alpha exponential of minus E a by R 0 T.

So, you see that this in the species equation when you write this, this is the omega i form and then this k come to in this temperature dependent. So, actually even though it is not apparent here where temperature arises of course, the temperature comes from here right. So, the reaction rate comes to end. So, constant the reaction rate constant contains temperature. So, that affects changed in the species mass fraction and that of course, you see that of course, temperature changes density also right and then this also, changes here. And you see that c j is essentially this species concentration and we can write this c j essential as in terms of mass fraction. So, this energy conservation the specific the sensible enthalpy actually couples with the species equations through this law of mass action term right.

So, this is how the coupling happens and further more when temperature changes the density also changes and then you have to consider the continuity equation and then all this things. So, of course, the flow also accelerate when the density changes because of this simple thing that you are continuity equation is nothing but d rho dt plus divergence of rho u vector is equal to 0. So, when the flow accelerates. So, when the density changes the flow also accelerates and of course, momentum also changes because rho u is equals to fixed right the flow also accelerates and that is happened due to a associated with the small change in pressure, but of course we have neglected the pressure here.

But here this gives an idea of how the coupling is happening that is very important at this stage to understand the this how the coupling actually takes place through this defined sets of equation, we are because our plenty of equation involved and that is very important to understand what each term represents, and how each equation is coupled to the other equation because if it was not coupled then I fill in a very simpler way would have solve separately, but that we cannot do that if we are solving if we are doing a CFD calculation of a combust or of a gas trouble engine, we need to solve all of this equations together. And of course, you note that this is for i-th species, so if there are if you have a if you have a 1000 species, then there will be 1000 species conservation equation and this will run from i is equals to N to that is i the summations will run then from i is equals to 1 to 1000 h i naught i naught.

So, this all the species the entire chemistry reaction mechanism that you see that is concentrated into this term and this term, where you need to some of or all the species to get the heat release rate contribution from all the species to get the heat release rate and we need to have the species equation for all the species that you saw then you will land up with 1000 equations. So, if you have 1000 species. Of course, with the mass conservation because of fact that summation Y i will be equal to 1 you need to solve for one less equation, but the total number of equations then you will have is that always essentially.

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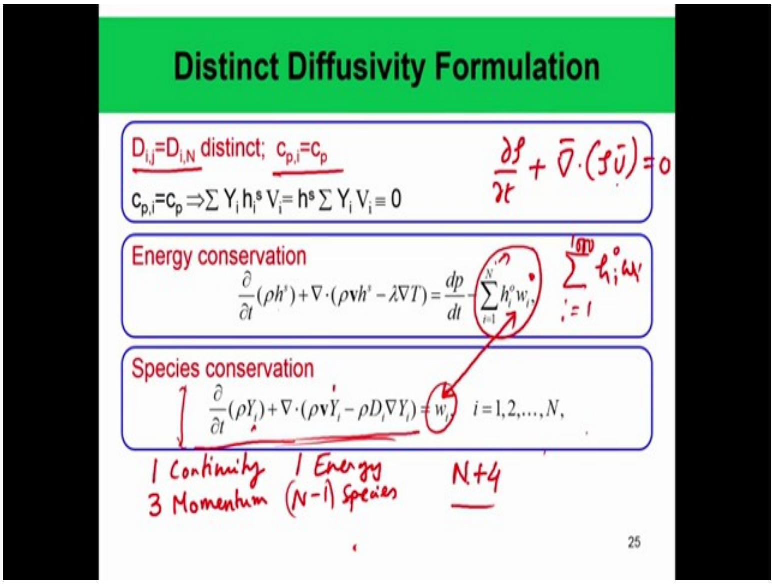

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$$\frac{\partial \rho}{\partial t} + \bar{\nabla}\cdot(\rho \bar{v}) = 0$$

Energy conservation

$$\frac{\partial}{\partial t}(\rho h^s) + \nabla\cdot(\rho \mathbf{v} h^s - \lambda \nabla T) = \frac{dp}{dt} - \sum_{i=1}^{N} h_i^o w_i$$

$$\sum_{i=1}^{1000} h_i^o w_i$$

Species conservation

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla\cdot(\rho \mathbf{v} Y_i - \rho D_i \nabla Y_i) = w_i \quad i=1,2,\ldots,N,$$

1 Continuity
3 Momentum

1 Energy
(N-1) Species

N+4

If you see we will have for to solve 1 continuity equation, 3 momentum equation, 3 because velocity is a vector momentum is essentially a vector one energy equation, but that energy will contain contribution from all this species i is equals to 1 to N, and then N minus 1 species equations depending on the number of species you have, and then of course, then you see that it is 2 plus 3 5, 5 plus N minus 1 that is equal to N plus 4.

So, typically for a large hydrocarbon like us in if you have likes say 10000 species then it will be 1004 equations partial 1004 partial differential equations that you need to solve. Now this looks very challenging of course, it is challenging, but then this is why it is. So, exciting and which is so complex and, but we need to understand it very detail level, because combustion as you see is very very important if you have to improve model engines, if you have to design new engines, if you have to make current engines more efficient in terms of producing more power more thrust and have greater efficiency.

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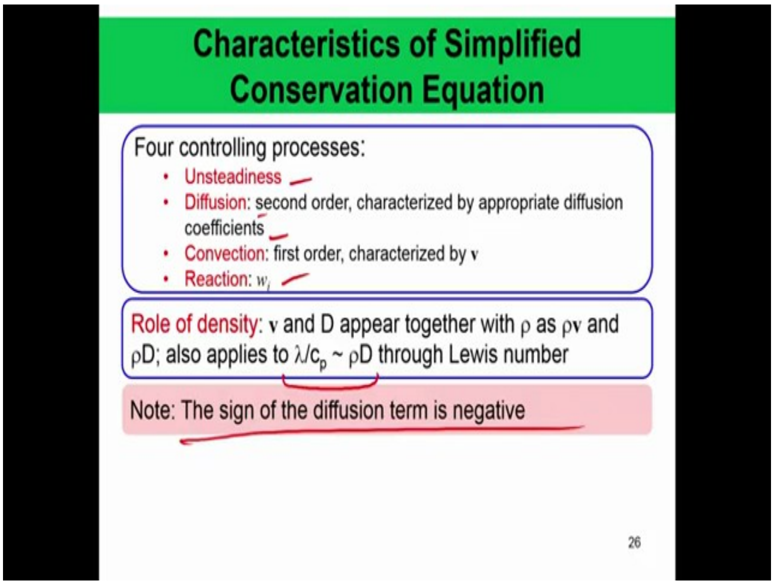

Characteristics of Simplified Conservation Equation

Four controlling processes:

- Unsteadiness
- Diffusion: second order, characterized by appropriate diffusion coefficients
- Convection: first order, characterized by **v**
- Reaction: w_i

Role of density: **v** and D appear together with ρ as ρ**v** and ρD; also applies to $\lambda/c_p \sim \rho D$ through Lewis number

Note: The sign of the diffusion term is negative

So, that is why it is very very important to understand them now. So, at the characteristic of the simplified conservation equation is that that we have retain the unsteadiness we have retain the diffusion, by diffusion we mean both species diffusion as well as thermal diffusion that is heat conduction and we have retain convection which is a first order quantity and of course, we have retained reaction and because combustion is represented by the reactions right and of course, it is a (Refer Time: 16:00) from the diffusion and reaction.

Now, density as we have seen that rho nu v and D appear together with rho and rho v as rho D and also applies through the Lewis number where as such if you see that in a combustion the density is a very very important we cannot has have absolutely assume density is constant, that is one very big difference. That is, these are not as such compressible flows in the sense that these are not high mark number flows that combustion can happen in low mark number.

Example: you have gas turbine engine combustion happen in a mark numbered of 8.1 0.1, 0.2 like something like that and the pressure inside a gas turbine engine of course, it is a combustion at a very high pressure 30 bar, but the pressure does not change at all in a gas turbine engine if pressure pressures changes very small, when compare to how it changes to the compressor how it changes to the turbine; if pressure changes very small inside the combustors, but temperature changes by huge amount, and because temperature changes the density changes.

So, we can assume it is like a isobaric flow of course, it is not actually isobaric even you solve for the momentum equation you need to retain your pressure if we are doing a c f calculation you need to retain your pressure terms, but it is close to an isobaric frame, but its strongly temperature variation varying flow the strong non homogeneity in terms of temperature rises as soon as you off the flame and of course, you have density changes. So, as soon as temperature rises the density also drops because pressure is constant. So, p is equal to rho r T if pressure is constant. So, density has to drop when temperature rises right.

So, these are this combustion flows are characterized by small change in pressure very large change in temperature, and very large change in density. So, these are the hall marks of combustion alright and then we will see related that also this change of density change of pressure change of temperature, no change of pressure, change of temperature happens in a very small regions in space and as well as such that is not effect of that arises, because your activation energy your activation energy is a very large quantity and that when your because of the nature of the reaction rate constant its essentially k is e to the power minus e a by r t.

So, when the when the activation energy is very large your temperature rises in a very thin and that is why flames are thin and that is why you have got very strong temperature gradients, that is temperature arise in a very small amount of time. So, that is why temperature gradients are larger when temperature gradients are large in diffusion, because you see diffusion is essentially arise comes as like a grad of rho lambda grad t. So, it is essentially del square t. So, essentially Laplace temperature is a Laplace in species mass fraction.

So, when temperature when the gradient are very large this del square and the second derivatives are also typically large in this region, and that is why diffusion becomes a very very important phenomena. So, combustion is essentially as you will see later within the flame combustion is essentially competition between diffusion not a competition it is essentially balance between diffusion and reactions right. So, and then that happens can be can happen in a flow that is convective also but they will come to these things later.

So, there then the of course, important thing is this the sign of the diffusion term is negative and that is arises because temperature change is heat flux changes from when you go from heat always flows from temperature high, high temperature to a low temperature region.

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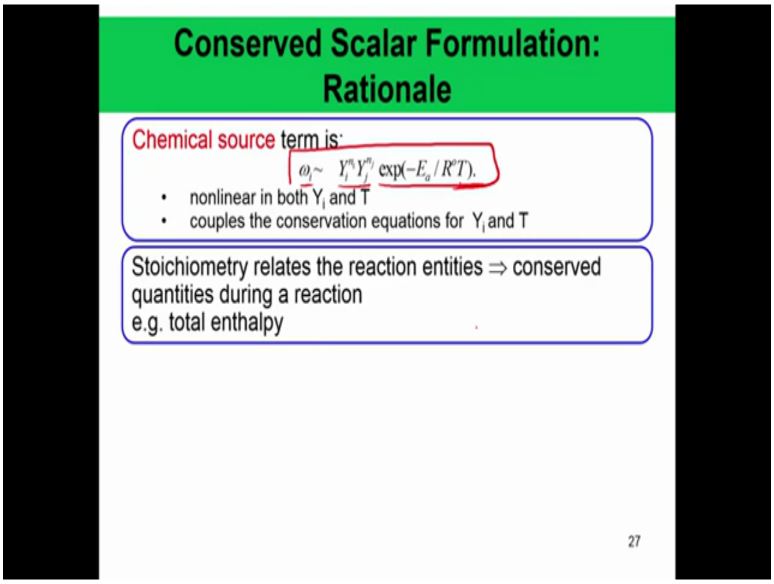

Conserved Scalar Formulation: Rationale

Chemical source term is:

$$\omega_i \sim Y_i^{n_i} Y_j^{n_j} \exp(-E_a / R^0 T).$$

- nonlinear in both Y_i and T
- couples the conservation equations for Y_i and T

Stoichiometry relates the reaction entities ⇒ conserved quantities during a reaction
e.g. total enthalpy

So, now the thing is that the chemical source term as you see that we can write it now as like in a terms of species mass fraction, if we have puts some constant in terms of molecular weight etcetera and then we can write the omega i then this is a reaction rate constant, is essentially Y i N j times Y j N j e to the power minus e a Y r 0 T is non-linear in both Y and T. This non-linear in Y because it is got exponent which are the stoichiometric coefficients, and it is non-linear in T, because of the e to the power of minus E by R 0 T and it couples the conservation equations for Y i and T.

So, this is a problematic thing because, it appears in both species equation as well as in enthalpy equation, but there is already non-linear coupling between both the species and temperature and the it also. So, this is one very big problem, that in both the species as well as in the temperature equations you have this reaction rate this chemical source term which can be either in terms of the species production rate or in terms of the heat release rate so, but dependents in this manner right it is a problem.

So, the problem can be circumvented by looking for something which such that we can somehow get rid of this, this chemical source term and for that the chemical source term what does it make what makes this quantities non conservative. Of course, as you see that h s is the specific enthalpy is not a conserved scaled and there is a Y i because it is for a source and the sink term respectively right. So, the idea is that we need to search for some quantities which is a conserved during a reaction.

Now stoichiometric reaction entities and that tells us that this conserved quantities they can be conserved quantities in a reaction for example, this total enthalpy. Now total enthalpy in a reaction what happens is that as you have seen chemically equivalent discussed about adiabatic flame temperature, this essentially enthalpy of formation going in to becoming sensible enthalpy when the reaction is complete. So, of course, then the total enthalpy does not change during is. So, then suggest that if we can be intelligent we are clever, we can find out quantities where which are essentially conserved.

Now, but the question is that it is very difficult to find out congruence which will be conserved in a convective diffusive medium. So, we can find out this quantities like a combination of different species mass fractions or combination of a of a species mass fraction and sensible enthalpy or total enthalpy which will be essentially total enthalpy. And we will see that in certain conditions we can make them conserved, but it will be very difficult to find something which is generically conserved which is generally conserved in a convective diffusive media.

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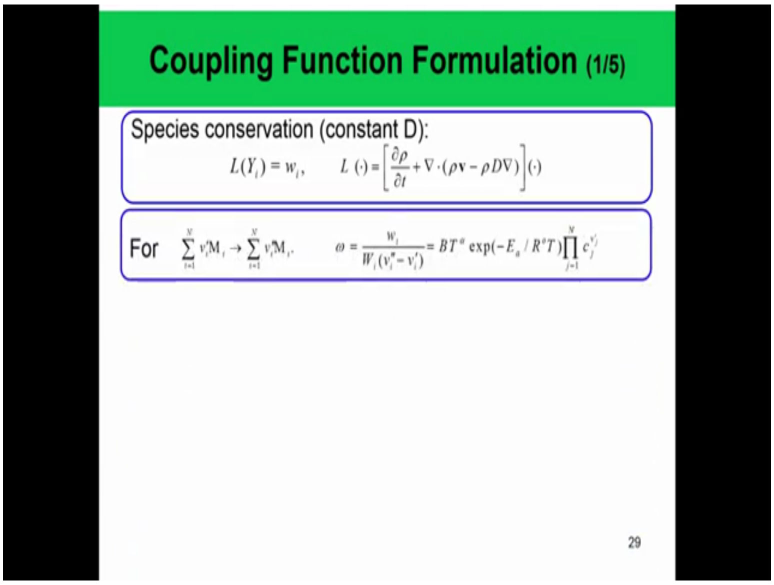

Coupling Function Formulation (1/5)

Species conservation (constant D):

$$L(Y_i) = w_i, \qquad L\,(\cdot) = \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v} - \rho D \nabla)\right](\cdot)$$

For $\sum_{i=1}^{N} \nu_i' \mathrm{M}_i \rightarrow \sum_{i=1}^{N} \nu_i'' \mathrm{M}_i.$ $\qquad \omega = \dfrac{w_i}{W_i(\nu_i'' - \nu_i')} = BT^{\alpha} \exp(-E_a / R^{o}T) \prod_{j=1}^{N} c_j^{\nu_j'}$

So if we will need to find out the coupling function formulations and we will go in to that. So, this as I said that the reason for the coupling function formulation arises because we have seen that both in the species equation as well as in the temperature equation, this chemical source term which is on the right hand side that has a non-linear dependence on both species mass fraction as well as on the temperature, of course, when you have non-linear dependence it is difficult to solve. So, of an more importantly that these appears in both species and the and the and the temperature equations which make them coupled, but you cannot solve them individually you have to solve all of them together because these are coupled through this things.

So, when you are now talking about the species equation to once again go back to this when you are talking about the if you this when you are talking about the if you talking about the energy equations say that is the if you are talking about the energy equation you have on the right hand side say this guy his total heat release rate and this heat release rate contains the species reaction rate the species production rate and the species consumption rate and each contains of course, it contains temperature, but it also contains the species mass fractions.

So, that is how this sensible enthalpy is essentially coupled to the species mass fraction, and when you consider the species conservation equation of course, you see that this also contains the species production rate obviously, it will contain the species production rate and the species consumption rate, but these also contains temperature through the reaction rate constant. This contains in this equation temperature is coupled to the species mass fraction through the law of mass action, because omega i is describes law of mass action where as Y i is coupled to temperature in the species conservation equation, because omega is also dependent on the reaction rate constant which is a function of temperature which is on (Refer Time: 24:47) dependent on temperature right e to the power of minus E a by R T.

So, this is how both this equation becomes strongly coupled right and of course, then it means that you have to if you have N species like the 1000 species of around 1000 equations together, and that two non-linear equations which becomes very demanding. So, what we do is that we formulate this something called a coupling function formulation. So, which will not contain this right hand side at all which will basically and so that we can basically solve this equation itself, and gain the required understanding of how the species in a temperature will evolve is it at also possible to do that we will see.