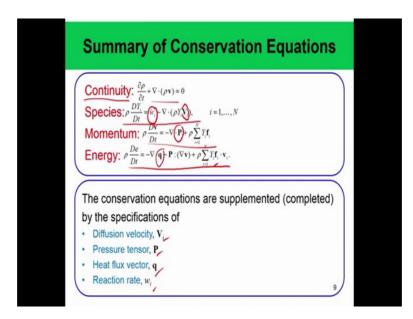
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Lecture – 15 Governing Equations III

Welcome back to this course on Combustion in Air Breathing Aero Engines. So, in the last class, we were discussing about the governing equations. So, as we have discussed of course, chemical kinetics in a very detailed manner and we have discussed how the reaction rate changes depends upon various factors like temperature species, concentration etcetera, but only that information is not enough because in a flowing system, in a practical engine; you have convection, you have diffusion and also you have other things you can how other things like radiation etcetera; which basically it means at the combustion parameters like species temperature this are also affected by the nature of the flow inside the engine.

So, to couple the flow on the properties like species concentration temperature; we need governing equations and you have seen that how using that Reynolds transport theorem, we can go from the description of a system to that of control volume and we have derived the governing equations for; we have obtained the governing equations in terms of conservation of mass which is the continuity equations and we have species equations momentum and energy.

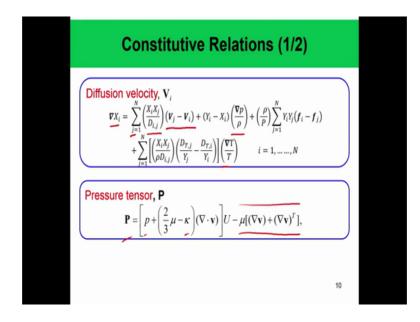
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And so these are the equations that we have as you see; we have obtained. We have obtained the continuity which is (Refer Time: 01:47) divergence of rho V is equal to 0; species equation momentum and energy equation of course, but as you see that these equations a are quite complex; even though they do not look. So, complex the thing is that many of this parameters many of this quantities like the diffusion velocity, like this quantity the pressure tensor, the heat flux body force etcetera; many of this are unknown and we need to provide auxiliary equations and consider derivation to close into solve the equations.

So, for that these are the things as we have seen that we need to supply equations for diffusion velocity, pressure tensor, heat flux vector and reaction rate and the this is a reaction rate of course, and which we need to which we need to basically close this equations.

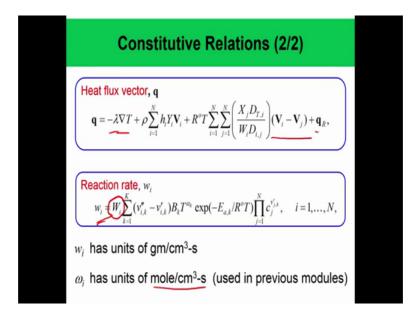
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And here is this diffusion velocity; now note there is a small connection with respect to previous class; this diffusion velocity which is actually implicit in terms of the species concentration gradient of X i, but here there is a summation from summation over j. So, that this gradient of X i for the there is a gradient of the species concentration of the of the molar concentration of the ion species gradient of X i; is essentially summation over j to 1; that is for all the species over than I; is given by X i, X j divided by D i j; which is a binary diffusion coefficient and which we obtained in the; if we remember in the previous transport of an (Refer Time: 03:18) phenomena class; there is V j; V i plus this things arising out of gradient of P gradient of T etcetera.

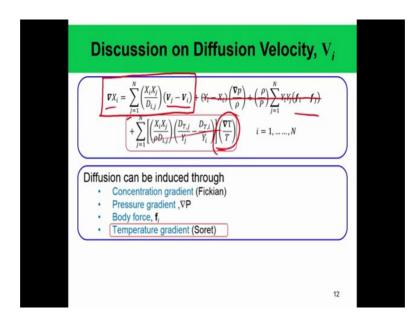
And of course this pressure tensor that we discussed; which is the standard description, so this is the pressure, this is the bulk viscosity and this is the string tensor which multiplied with dynamic viscosity gives you the shear stress basically.

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And also the heat flux vector; we have discussed which also comes out mainly from conduction gradient of temperature; this is the thermal conductivity then also the heat flux vector can be affected through the different heat content of different species and also due to temperature also due to molecular diffusion velocity and of course, heat radiation. And then we have of course, discussed reaction rate in great details and this is the reaction rate formula that you see and of course, one point important point to notice that these is units of gram per cubic centimeter; whereas, in the kinetic class we obtained reaction rate in terms of units of mole per cubic centimeter and this is the difference that arises that we need to take into account the molecular weight of the species.

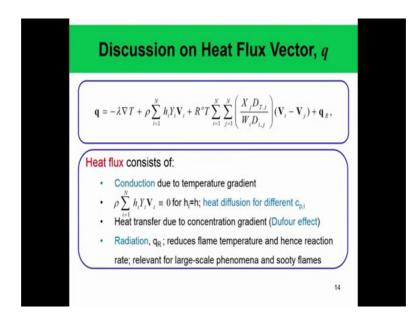
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So once again not here there is a correction the summation over j summation goes from j equal to 1 to N; instead of I equal to one to N. So, one this thing is that of course, this means that this gradient of this the concentration which can arise due to this difference of the species diffusion velocities V j minus V i and due to pressure gradient and due to body force difference and due to temperature gradient.

Now, these are typically negligible in; we will neglect this unless other unless this specific situation arises, but mostly we will neglect this and can combustion of our discussion; this is also typically negligible that this is a Soret effect. Now, arising out of temperature gradient and we will discuss this in great detail, so we will mainly consider that our species diffusion will mainly we concentrated in to this region and we will neglect all this things; unless are mentioned.

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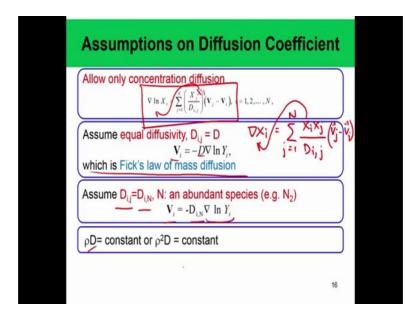
So, these are the different things out of temperature gradient, pressure gradient body force and concentration gradient and temperature gradient etcetera. Now, we will go just we have already discuss this; so, we will not go into this different things; how the heat flux vector changes.

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Auxiliary Relation	
Ideal Gas Equation of State	
$p = \rho R^{\circ}T / \sum_{i=1}^{N} X_{i}W_{i} = \rho R^{\circ}T \sum_{i=1}^{N} \frac{Y_{i}}{W_{i}} = \frac{\rho R^{\circ}T}{\overline{W}},$	
Energy–Enthalpy Relation	
$h=\sum_{i=1}^{N}Y_{i}h_{i}=e+p/\rho.$	
Calorific Equation of State	
$h_{i} = h_{i}^{0}(T^{\circ}) + h_{i}^{*}(T;T^{\circ}), i = 1,, N \qquad h_{i}^{*}(T;T^{\circ}) = \int_{T^{\circ}}^{T} c_{p,i} dT.$	
Mole and Mass Fractions $X_{i} = \frac{Y_{i}/W_{i}}{\sum_{j=1}^{N} Y_{j}/W_{j}}, Y_{i} = \frac{X_{i}W_{i}}{\sum_{j=1}^{N} X_{j}W_{j}}.$	
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This is just a recap which we will not and of course, we need the auX iliary equations like P, we need the equation of state, we need the energy enthalpy relations and of course, remember the total energy that we discussed is essentially the sum of the enthalpy of formation plus is the sum between the enthalpy of formation at temperature T 0; plus the sensible enthalpy at temperature T with respect to the reference temperature T 0 and of course, this sensible enthalpy can be written as integral T 0 to 2 times c p i; where c p i is a specific heat of the ion species times d T.

And then of course, we frequently we need to convert between mole and mass fractions because the species equation is given in terms of mass fractions. Whereas your reaction rates are retained in terms of mole fractions, so here is how you convert it X i is equal to Y i divided by W i divided by summation j is equal to 1 to N; Y j by W j and this is the how to convert from mole fraction to mass fraction, so these are the things.



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And then we simplified that if we assume that this is we only consider this the only consider the gradient can arise due to that only if we consider the concentration gradient effect on diffusion. So, this is what we are basically have left with here you see that X i the X i was here. So, the X i has basically spins it is summation over j, so the X i has come over here. So, we actually equation was gradient of X i is equal to summation j is equal to 1 to N; X i; X j divided by D i j times V j vector minus V i vector.

So, if since this we have neglected other terms, now the X i can escape this thing and it can come over here. So, when it comes in the down stares in the denominator it becomes log of X i and now one can apply several simplification that if you can apply equal diffusivity is then it is become simple and then you can write it explicitly V i is equal to

minus T lon minus D gradient of logarithm; natural logarithm of Yi and this is the fixed law of mass diffusion.

But better assumption is that we instead of equal diffusivity, we consider that D i j is equal to D i N, where N is the abundant species and this is a good assumption because you see that that of course, in air we are considering air breathing combustion in in situations when the oxidizes air instead of pure oxygen. And when there is air the abundance species of course, nitrogen which is about 71 percent by volume in air and of course, its fuel mass fraction is very small and the oxygen mass fraction is mole fraction is also small 21 percent by volume and so mainly it is nitrogen and so we can think that all the species whether it is a fuel, whether it is oxygen; it is basically diffusing in a sea of nitrogen essentially. So, we can consider that is D i j is essentially; D i N, where N is the abundant species which is for a chemical nitrogen and then we can write that that V i is equal to minus D i N where N is; this D is basically the D i N is essentially diffusivity of ion species with respect to a N; N X species which is abundant species and then this becomes gradient of lon Y i.

And then we depending on the situation we assume that rho D is equal to constant or rho square D is equal to constant and this will calculate later.

Isobaric Assumption
Relevant for subsonic flows $\begin{pmatrix} \frac{du}{dx} = -\frac{dp}{dx}; \\ \frac{du}{dx} = -\frac{dp}{dx}. \end{cases}$
Let $\hat{p}(x,t) = \hat{p}_{0}(x,t) + \hat{p}_{1}(x,t)$ $\hat{p}_{o} = O(1)$ $\hat{p}_{1} = O(M_{o}^{2}).$ $O(1): \frac{d\hat{p}_{o}}{dx} = 0$ $O(M_{o}^{2}): \gamma M_{o}^{2} \left(\hat{p}\hat{u}\frac{d\hat{u}}{dx}\right) = -\frac{d\hat{p}_{1}}{dx}$ Therefore $\nabla \hat{p}_{o} = 0$, or $p_{o} = p_{o}(t).$
$p_0(t) = \rho RT = \text{thermodynamic pressure}$ $p_1(x, t) = \text{dynamic pressure}$
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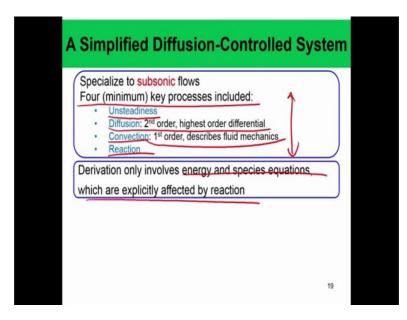
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And we have also go on our isobaric assumption which by which we showed that the for subsonic flows essentially; we can consider this equation itself because the equation between reacting and the non reacting for the momentum equation; this is essential, the momentum equation is not different because momentum is essentially conserved in chemical reactions and the only difference is that when you have reacting flows; the density changes. So, that is how reaction reacting flows differentiated with respect to non reacting flows; at least in terms of the momentum equation.

But what I want to say here is that the order of one acceleration, you only need an order of mach number square of pressure gradient and as a result your pressure is essentially the spatially is essentially constant within your combustor. It of course, drops for little bit for in subsonic flows and it increases in supersonic flows. For example, this in a gas turbine engine you have a small pressure drop downstream in the combustion region that is in the product gases.

Whereas in scramjet combustion, you see that you will have essentially little bit of pressure rise in the combustion gases; in the product gases essentially. So, then we have considered this is the background pressure P 0 is equal to the rho R T and P 1 X T is equal to the; it is a dynamic pressure.

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And then we need to basically what we have to do here is that; we want to derive simplified set of equations of diffusion controlled systems and we will do that here. Basically, let me just do the derivations this is important and so that this is the assumptions that we will specialized to subsonic flows only and only 4 minimum key processes will be included.

So, we will include unsteadiness; we will include diffusion that is the; we will include the mass and then we will include species diffusion and we will include thermal diffusion that is conduction. We will include convection and of course, we will include reaction because otherwise if we will then include diffusion and reaction then it does not really the; solve out real combustion situation.

As we will see that in certain cases we will be able to neglect convection not of course, inside an engine, but when we are discussing about; I want a simplified system for example, in a one dimensional non premixed flame or a one dimensional premixed flame, we will be able to neglect convection and essentially competition between your reaction and diffusion and that we will come later.

But anyways so, but we will not go there right now, we will just have this four processes included unsteadiness, diffusion, convection, reaction and we will see that the derivation only involves energy and the species equation which are explicitly affected by reaction. So, basically the thing is that as we have seen in last class and today also that in the low Mach number limit; your pressure really does not change and as a result, your pressure gradient is very small.

So, your momentum which is rho U times; U even though that changes by small amount will this does not really; we will consider a very simplified point of view from momentum. So, that whatever the gas accelerates that can be computed through the continuity equation and there is no really change of momentum if the pressure gradient is small.

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Isobaric Assumption
$ \begin{array}{c} \textbf{Relevant for subsonic flows} & \textbf{O(1)} \\ \rho u \frac{du}{dx} = -\frac{dp}{dx}; & \left(\frac{\rho_s u_s^2}{p_s}\right) \left(\hat{\rho} \hat{u} \frac{d\hat{u}}{dx}\right) = -\frac{d\hat{p}}{dx}; & \gamma M_s^2 \left(\hat{\rho} \hat{u} \frac{d\hat{u}}{dx}\right) = \left(\frac{d\hat{p}}{dx}\right) \end{array} $
Let $\hat{p}(x,t) = \hat{p}_0(x,t) + \hat{p}_1(x,t)$ $\hat{p}_o = O(1)$ $\hat{p}_1 = O(M_o^2).$ $O(1): \frac{d\hat{p}_o}{dx} = 0$ $O(M_o^2): \gamma M_o^2 \left(\hat{\rho} \hat{u} \frac{d\hat{u}}{dx} \right) = -\frac{d\hat{p}_1}{dx}$ Therefore $\nabla \hat{p}_o = 0$, or $p_o = p_o(t).$
$\rho_0(t) = \rho RT = \text{thermodynamic pressure} \\ \rho_1(x, t) = \text{dynamic pressure}$
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So, we will do there is actually; if you see that that can be essentially explained from this isobaric assumption that once again; if we go back this, but in this non dimensionalized form; if you have to change and create an acceleration of order 1; this pressure gradient will be order of mach number square that was the thing and so of course, the flow accelerates in a reacting flow as you see.

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Derivation (1/2) Energy conservation In terms of total enthalpy, h; $\rho \sum Y_i h_i (\mathbf{v} + \mathbf{V}_i) - \lambda \nabla T$ 20

But then this we will consider that this acceleration can be computed essentially through the continuity equation for the system that we will consider and momentum equation will not be really discussed explicitly in our derivation. So, this derivation we will only include the species equation and the enthalpy equation and enthalpy equation we will see that it does not come explicitly. We will actually start with the internal energy equation that we have derived and then from the internal energy equation, we will combine this with the species equation to arrive at the enthalpy equation; so, that is what we are going to do first.

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$$Derivation (1/2)$$

$$S \frac{De}{DE} = \frac{\lambda}{\lambda E} (Se) + \overline{V} \cdot (S\overline{V}e) = -\overline{V}\overline{2} - P : \nabla V + S \frac{\nabla}{2} + S \frac{\nabla}{2}$$

So, the equation that we have if you see the equation that we have derived previously was this; this is the rho times D this is the material derivative D e; D t is equal to partial dou derivatives of with respect to time over rho E; plus divergence of rho V vector, this is a small v vector; that is a bulk fluid velocity, times the internal energy is equal to minus of grad q; minus P V this means that the tensor has to be counteracted twice plus this is the diffusion velocity.

Now, what are the terms we can get rid of this of course, we assumed that is in a body force; so, this goes to 0, this can be shown to become simply P times divergence of V let us now P is a scalar essentially. So, then this becomes whereas, q vector that is a heat flux vector is equal to minus lambda grad T; is a conduction term plus rho times summation i is equal to 1; to N time Y i; V i this is a species diffusion velocity. So, this is as you see that we have left out lot of things, but this is the most simplified form of heat flux vector that we can write at this stage.

And of course, as we have seen that the V i is given by if it is a simplified system, if you use fixed law of mass diffusion it is given by V i vector is equal to minus D i with respect to N times gradient of X i. So, that is how V i can be given or if you want to use the full bad diffusion equation, you can write the gradient of X i is equal to summation j is equal to 1 to N; X i, X j divided by D i j times V j vector minus V i vector also.

Now, what we can do is that; we can write E that is the internal energy is equal to h that is the specific enthalpy minus P by rho; that is a definition of enthalpy h is equal to that is E plus P by rho of course, this is specific quantity.

And then if you substitute this into here and write that h is equal to summation bulk specific enthalpy is equal to summation Y i; h i is equal to 1 to N then this hints that is this is a transient term dou dou T of rho times summation Y i; h i plus this is the gradient of brackets density times summation Yi; h i plus V vector plus V i vector minus lambda grad T. I will explain this term in second is equal to d p dt. So, this is the transient term this is the basically the convection term and this is the species diffusion term and this is the heat flux crossing the boundaries this is also the heat flux crossing the boundaries and that is carried over by the species diffusion velocity, this is the flux crossing the boundaries due to temperature gradient and that is equal to dp; dt.

So, this is what we have derived, but you see here interestingly there is no reaction rate happening. So, how does the when does a reaction rate coming; if you want a you can sphere also you can just pause here and just think where does the reaction rate can actually come from the clue is that you remember that this is total enthalpy. So, total enthalpy of course, contains as we have seen that the total enthalpy h i is nothing, but h i 0; that is the enthalpy of formation plus h i sensible. So, these two things so now, you can think that where does the reaction rate can come from.

And of course, when you have invoked this is not enough; now we need to also include the species conservation equation in these forms now. So, this species conservation equation is given by this is of course, the energy equation and this is the this is the transient term and this is the essentially it will contain the convection term of the species Yi; V vector species converted into the bulk frame velocity plus the species crossing the control surface of the element here; due to the species diffusion velocity V i capital V i and that is equal to the reaction rate term. Once again this is W i not omega and this is goes from i is both equations go from i is equal to 1 to N.

Now, what we can do is that; now we can multiply this equation on both sides by h i 0 and then sum over; sum over from. So, this is multiply this equation with h i 0 and then sum over i is equal to 1 to N. If you do that; what we will get is that, so what we have done is that we have derived the enthalpy equation and we have also in a simplified form we have derived the enthalpy; the total enthalpy equation from the internal energy equation and we have simplified it in terms of the; we have neglected some of the terms, we have got a simplified definition for the heat flux vector that is crossing the element surfaces essentially, element boundaries and then we have obtained the species equation and that is also in a simplified form and then we have sum over from i is equal to 1 to N.

And this new species equation that you get; if you subtract from the previous enthalpy equation the total enthalpy equation; we will get, what we will we get? We will get the equation for the sensible enthalpy. So, you have a just to give you one example; we have we have got an equation for the governing equation for h i total and then you have got an equation for h i 0 and this is obtained by h i multiplying h i 0 times Y i.

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And then the governing equations for that and then this was a governing equations for h i S and then if you subtract these two things, if we subtract between this two things what

we are left with is essentially the equation for h i S because h i is; S is nothing, but h i minus h i 0.

So, what you get is essentially you can you should do the derivation yourself and just write down the final answer here; that is the equation that you get is nothing, but this one density this is a very important equation because this is the equation that we use for all of our combustion calculations and this is also the equation either this form or the temperature form that appears. So, this is the convection term plus there is rho times summation i is equal to 1 to N; this is once again the enthalpy the sensible enthalpy that is crossing the system boundaries due to different species due to different; actually we will see that this is due to different specific heats; minus lambda T is equal to dp, dt minus now we will see the magic i is equal to 1 to N.

This is nothing, but the heat release rate why; this is a reaction rate, this is species consumption rate and this is the enthalpy of formation. So, when you are sum over i is equal to 1 to N, you essentially get the heat release rate that we will see and this is what is actually change in actually increasing the sensible enthalpy before and after the reaction with respect to the state previous to the reaction.

So, this is our very important governing equations that is the species enthalpy equation and of course, here h S is nothing, but summation i is equal to 1 to N; Y i h S i. So, this is the species enthalpy equation that we have derived, so this is how you go from the internal energy equation to a sensible enthalpy equation and I strongly encourage all of you to interest at derive this equation yourself; it is not very difficult at all.