Combustion in Air Breathing Aero Engines Dr. Swetaprovo Chaudhuri Department of Aerospace Engineering Indian Institute of Science, Bangalore

Lecture – 14 Governing Equations II

Welcome back. So, we were talking about governing equations for chemical evacuating flows that is a combustion flows involving combustion, and we arrived at the equations for conservation of mass momentum species and energy. And we found out that while those equations were complex in itself it was not closed in that is several of this things like reaction rates, like species diffusion velocity, like pressure, like heat flux vector q, these things needed supplemental information or auxiliary information or auxiliary equations or constitutive relations as such to basically close these equations.

So, first things first that is we need to understand what is species diffusion velocity.

So, if we look into that this is the species diffusion velocity V i that is essentially given in a very implicit complex form and this is given as this in this equation this is the gradient of the species mole fraction it is a gradient of X i is given like this, where this species

diffusion velocity V i appear also note that this species diffusion velocity V j appear and also there are several other things appear.

But this is the most important part you see where V i appears also gradient of pressure appears body force is appear gradient of temperature appears also right and but we will we see that we will mainly focus on this and we will tell you what the other things like these are extra are, but this is the main point of our will be the point of our focus and we will simplify this to arrive at simpler equations, but this is the most generalized form we need to know the most generalized form and then you need to know how to arrive at a simpler form because otherwise your knowledge will always be partial.

So, you will always as you know that it though it looks complicated and though it looks involved, we will start with the full complex form and then we will simplify this to arrive at a generalized form and these simplified forms will be used for further analysis of different kind of flames and combustion systems. We should concern yes as you know that first is this of course, this pressure terms are consists of this thermodynamic or pressure P and plus of course, this can actually have thermodynamic pressure dynamic equation we will come to that, but essentially this also contains this viscosity and the velocity gradients.

And then also we will see that this contains a bulk viscosity that is kappa or and this will be only important high speed flows and we will not be, but it not in a high speed flows it can be important, this is the difference times this velocity vector that you come here and this is actually you are the strange things that we see come, and this is the dynamic velocity part that we are fairly come on in fluid mechanics.

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So, this will essentially we say that it can be able to neglect this part, and heat flux vector as we will see that this heat flux vector is given by this is the thermal conduction terms this is the thermal conductivity, and this is essentially the enthalpy transport this is the heat flux that is arising due to different heat contents and the diffusion velocity.

So, diffusion velocity is can also cause thermal transport and this is essentially as we will again see that this is a kind of a heat flux due to once again due to diffusion velocities and they arises due to due to this difference of the species diffusion velocities, and also there can be a radiation term that is the from q radiation.

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So, and, but most importantly and of course, these are the important, but the most important thing in combustion in this constitutive relations of course, the reaction rate that is omega i. So, this reaction rate you see that we have they cannot be reaction rate in this form that is omega i this is w i the difference is this molecular weight w i, because this equations as you see is written in rho i that is the density of the ionex species or the mass fraction of the ion (Refer Time: 04:30) species zone that is why this small unit change come, this note that please note that this units of our small w i has grams per cubic centimeters per second where as units of omega i that we discussed previously for which we derived this law of mass action, that is omega i is essentially is equal to nu double i double dash minus nu i dashed, times K times product of j is equal to 1 to n c j times nu j dashed this things that we discussed.

So, this is the difference is this w i which is a molecular weight otherwise everything is same. So, now, of course, this was a true if we considering only one step reaction, but then when there is the contribution from this from omega i can come from k reactions. So, we need to consider all the reactions and this is the most generous form, and as you remember the these part of the equation is nothing but our reaction rate constant for the kth reaction, and these another part this was essentially the law of mass action. So, with this we could write this reaction rate form which is not very difficult.

So, once again I am emphasizing that we are writing a generalized form, because this will give you an idea of what everything that goes into this into combustion and then we will simplify it do not do not do not worry about that.

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So, discussion now if you discuss this what goes into the diffusion velocity that is if we go back to this equation that is gradient of this x i was given by this thing is given by this summation i is equal to 1 to n x i times x j divided by D i j times V j by. So, we were discussing the diffusion velocity and this is the gradient of x i is equal to summation given is equal to this thing where you see diffusion velocity of the species i if you are interested in that and of course, that is dependent on the gradient of the of x i which is a gradient of the mole fraction of the species i, but then that is also committed to several things it is an implicit equation that you gave and this is of course, as I said binary diffusion coefficient D i j and, but the velocity of the j-th species are also involved and there are several other things.

So, this first term is essentially comes from the concentration gradient, this tends the Fickian diffusion term essentially. So, the concentration gradient that is this is the Fickian diffusion terms this is a concentration gradient and of course, you see that there can be a pressure gradient also can gives this thing, and there can be a body force

gradient body force that is involved here and then there can be a temperature gradient that is a Soret effect which we found that to causes a counter gradient diffusion of hydrogen or soot like species or heavy species respectively, but the most important term is this one and we will come to this. So, this is the concentration gradient term, this is the pressure gradient term, this is the body force term and this is the temperature gradient term which is the Soret effect.

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So, now pressure we have discussed in a fluid mechanics test of course, we have we can discuss we can discuss fine more about this in a fluid mechanics course, but of course, the gradient of pressure in a the main force that drives fluid is the gradient of pressure. And then there the acceleration term is essentially the then the left hand side what you see this convective terms time on the convective the temporal term, and the convective term these are like temporal acceleration and special acceleration respectively. And then you can have viscous forces which are like due to this the if you coming from the viscosity times d o dou 2 u dou u square this sort of things.

And, but here the additional complexity is that there is temperature enhance density variations on in an the bottom flames constant density is a poor assumption and buoyancy effect is inherently important and role of electromagnetic force body force is not petty clear ok.

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So, we will not discuss much about this, but typically what we will see is that in we will see later also that we do not pressure yes of course, it drives the fluid it is used for understanding the overall flows of the system, but in combustion at least in subsonic combustion the pressure changes small, but the if the pressure can become very important when you have certain dynamics inside a combustion like thermal acoustic oxidations, which is self exerted oxidations creating large fluctuation in pressure any ways. So, we come back to the discussion on the heat flux vector q vector.

So, this heat flux vector or heat flux can cross this control surface because of temperature gradient conduction due to temperature gradient, this is essentially the heat transfer due to different heat contents of the different species and this heat diffusion for different c p i it will be we will see that when this the different cps, that is the specific heats of the of the different species at different then this term will be important. But when this is when all specific heats are essentially can be considered in to an average specific heat or when this or when there we will use a constant specific heat for all species then this will becomes to 0.

And then there can be concentration due to heat transfer due to concentration gradient which is Dufour effect which is not so much importance, we will not really consider this and then there will consider radiation of course, that can be important and especially it is important in flames which involves lot of soot because as we discussed that soots are essentially black body black bodies, and this soots emit radiation which are like similar to that of a black body radiation. So, in those cases suppose in a combustor we have strong non (Refer Time: 10:50) combustion if we have a strong soot emission that can reduce the temperature of the flame and that can cause lot of heat flux into the combustor walls also.

So, this lot of things we need to consider depending on the situations. So, once again this is the heat flux due to the conduction which is due to temperature gradient this is the due to different heat contents and this is heat transfer due to concentration gradient, that is a Dufour effect and the radiation q r they can also become very important, but this can be actually very complex and to calculate, but typically found (Refer Time: 11:24) flames or lean femings flames are which does not involve much soot we really do not we will not really also consider this radiation as such, because those radiation is not of much importance, but understand that in sooty flame this is very very important.

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But you of course, is very much situation dependent on which situation we are talking about all right. So, another thing is that very important is of course, the auxiliary equations there is a ideal gas equation of state P is equal to rho times R 0 T , R 0 is a universal gas constant and these things downs to (Refer Time: 12:00) is very important that is the mean molecular weight. So, essentially P is a P is equal to rho times R 0 times T divided by mean molecular weight, and mean molecular weight is nothing but summation i is equal to 1 to n x i, w i, x i is a mole fraction and this is also equal to summation i is equal to 1 to n y i mass fraction by the molecular weight inverse ok.

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So, this is the mean molecular weight formula which is which will come very handy when you want to calculate something like pressure from a given data set etcetera or you want to estimate pressure in the equation.

So, then energy enthalpy relation Y h that is a specific enthalpy is nothing but the sum of the enthalpy times their mass fractions enthalpy Y i times h i, Y i is a mass fraction of the species i inside the system, and h i is the is the specific enthalpy of the ion species and of course, that is equal to internal energy plus P plus P y rho. Now the most important thing as we have discussed is that this h i this specific enthalpy consist of two parts, this is enthalpy of formation which is defined at T 0 and it is actually contains the total bond

energy of the total essentially the heat of combustion is carried into this enthalpy of a formation which is the total enthalpy of the products minus total enthalpy of the reactants and this is the sensible enthalpy that is the enthalpy of this at a temperature T with respect to T 0 ignore that this enthalpy of formation is defined at T 0 the reference temperature.

So, the enthalpy sensible enthalpy can be written as integral T 0 to at a sensible enthalpy at temperature T with respect to the reference temperature T 0 can be can be written as integral of T 0 to T c pi d T, where a c p i is the specific heat of the ion species integrated over temperature, and this is very important conversion between mole and mass fractions. So, the conversion this is very very important when it comes extremely handy in different situations. So to given; if you are given mass fractions Y i and you need to convert to mole fraction x i you need to know the molecular weights of the different species involved and the x i that is the mole fraction of the ion specie is nothing but the mass fraction of the ion species divided by the molecular weight of the ion species divided by summation over i equal to 1 to N, Y i divided by W i . So, it is a summed over all the species.

So, that is the thing and if you are given mole fraction and you want to convert to if you are given mole fraction and you want to convert to mass fractions this is also very important because there is given by X i times W i divided by summation j is equal to 1 to n x j y j. Now why this is very important because you see in combustions; if you consider the species equation say you are basically deriving the equation for the mass fraction on the species i. But then you go to law of mass action then you have the on the right hand side you have the reaction rate and the reaction rate of course, it contains of the law of mass action which is that k the reaction rate constant times the product of the concentrations of c j times the nu j, that is a stoichiometric coefficient raise to the power exponents

So, this cj is actually essential in concentration which is typically comes in moles mole fractions right that is a moles per cubic centimeter or we can convert that from mole fractions. So, those are in essentially units of moles. So, from that in the this species equation itself we have this two different kinds and you need to understand the conversion factors of the conversion methods to come from one from mole fraction to mass fraction or mass fraction to mole fraction.

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Now, as we said that when you do diffusion we will neglect all other effects in the for these further this class and we will arrive at the simplified formula for diffusion, and this is given by gradient of this also what we have taken is that we have just taken this if we go back to this complicated formula for diffusion, if we remove all these things now we what we will do is that we will just remove this part and just remove this part and we will only focus on this part right. And once we focus on this part we can essentially take what we can do is that, we can we will see that we can simplify this part even more and we can write this as this form which is given by log of gradient of this log of X i is nothing but summation *j* is equal to 1 to n x *j* divided by D *i j* which is our diffusion coefficient or which the formula of which we derived in just in previous class in transport phenomena either from collusion theory or from using the kinetic theory n times of vj minus vi ok.

And then if we assume that there are equal diffusivities then the problem becomes even more simplified, that which is not a very good assumption in combustion because any ways then D j is equal to D then this essentially goes out and you have we got an explicit relation for V i which is nothing but minus D lon of y i which is the Fick's law of mass diffusion. And then better assumption is that this is this is not a good assumption, but we assume all this equal diffusivities, now better assumption is that we assume that $D i j$ is

equal to D i N where n is an abundant species, but this is a better assumption because when we consider air breathing combustion that is combustion in air of course, the abundant species nitrogen. So, we can assume that all are we will not consider the all diffusivities, but we will also only consider that that are the species i diffuse in a bulk environment which is D i j is equal to D i n and this bulk environment is mainly composed of nitrogen. So, then this will xms this is basically d i n and then we can write this V i that is a species diffusion velocity of i on this i th species diffusion velocity is nothing but minus D i n instead of D term i simply write D i n of lon i.

So, yes this was one instead of this D i j storing all this D i j and we are storing one. So, that was very cheap computationally in expensive, but this is little more expensive we need to store instead of i j n cross n cross n we need to store basically n. So, it reduce the dimensionality of the problem, but still this is much better and, but then assumption is that we assumed rho d is equal to constant or rho square d is equal to constant depending on the situation.

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Now, before we go in to this now we need to talk about something we are talking about this thing that is the pressure we need to have a some discussion on pressure, but we want to show that in general the pressure inside this inside a combustion system or any system as such when their Mach number is small, that the pressure variation is small and we will talk about in this class is except for scramjet combustion our Mach number will be small and this we can consider we will show that pressure does not change too much inside a combustor. Actually it decreases slightly instead of a subsonic combustion and that leads to the slight reduction of the thermal efficiencies as we know, but the pressure drop is actually small.

Now, why is it small and because of pressure drop is small we can consider this to be a constant pressure process, but we need to show why is it so? This is a very very important in the key assumption in combustion that goes on, and you see in reality it cannot be using it is not possible for pressure to be constant, because whenever there is a flow acceleration of course, there has to be a pressure change because it is a acceleration and there is a force, but as we will showed that even when for large acceleration the amount of pressure drop required is very small. So, and here of course, in combustion the acceleration of the fluid basically comes from the heat release.

So, what I were talking about is let us suppose about why (Refer Time: 20:37) talking about flow acceleration or suppose we write the continuity equation rho times u, rho 1 u 1 is equal to rho 2 times u 2. And suppose this we have -[pro]duct and we have a flame like this and this is rho 1 u 1 and this is rho 2 u 2, rho is the density u 1 is a velocity and upstream velocity this is the downstream velocity and this is the flame and of course, because this density is small your u 2 is large. So this is cause, this is the flow acceleration. So, this flow is now accelerating with this flow.

Now, but then the question is that does this mean how much this flow acceleration, how much pressure drop does this required or does this cause that the we want to show that that is not large, and you see as such in the momentum equation your pressure appears this as a because in a momentum equation your gradient pressure is the force and your left hand side is essentially the acceleration. So, for acceleration there is this gradient of pressure is as to be non zero, but we will show that this is small right that is the purpose of this exercise. So, let us go in to that.

So, for that we will we will consider just a one dimensional flow and we were discussing this what we are discussing here that is this rho 1 u 1 and this is the flames rho 2 u 2 we will discuss this in a small elementary form in a by rating in a ordinary differential equation. Now we one thing is that in the momentum equation in chemical reactions momentum is essentially conserved.

So, in a momentum equation you do not have any idea whether there is reaction or not except for the fact that the density changes and the density changes causes of acceleration using continuity, and that acceleration is has to reflected in the momentum equation right. So, except that there is no explicit chemical reaction happening inside a momentum equation, so anyways. So, we will consider if we consider this one dimensional equation momentum equation this is the equation. So, it is rho if you write the one dimensional momentum equation with removing all the complexities we can just write it like a rho times u times du dx, this in a steady state of course, that is why you do not have any transient terms is equals to minus dp dx. So, this is the way.

Now, let us consider that you define non dimensional variables U cap is equal to u by u 0 we define rho cap is equal to rho by rho 0, these are like some reference variables we will come to this soon and P cap is equal to P by P 0. So, now, if you do this in cooperate this one dimensional equation inside that we will find that you will get what you will get this rho 0 u 0 square u cap, d U cap dx and here you will get minus P 0 d P cap d x. So, rho 0 u 0 square by P 0 u times is U cap du dx is equals to minus d P cap dx.

Now, you if we write we can write P_0 is equal to rho $0 \rceil$ right this is the actual gas constant your particular gas constant and we can write P 0 by rho 0 is equal to r. So, P 0 by rho 0 is equal to r T and we can multiply with gamma on both sides then this becomes essentially is equal to some speed right this is c 0 square. So, then what we can do is that if we multiply by gamma here gamma here then this equation becomes then this equation essentially will become gamma times u 0 square by c 0 square is equal to sorry times U cap du cap dx is equal to minus dp cap dx.

Now, let us remove this and then this becomes gamma times Mach number squared right and then this is U cap du cap dx is equal to minus dp cap dx. So, this is non dimensional acceleration this is non dimensional pressure gradient. So, what does this tell? This tells that if you want to change if you want to create or acceleration by order 1. So, this if this is an order 1 quantity you need to have a pressure gradient or the of the resulting pressure gradient which will happen depending on the situation is order Mach number squared. So, the pressure drop that you get in combustion from an order one acceleration of the flow is order Mach number square. So, if the Mach number of the flow is small typically Mach number in subsonic combustion in a gas turbine is 0.1 to 0.3, it is order Mach number square is a 0.1 times 0.1 minus 0.01. 0.3 times point three means 0.09 ok.

So, the pressure drop becomes very very small, as a result we can essentially neglect the pressure drop in side a subsonic when there is subsonic combustion ok.

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So, this what we have understand that for subsonic flows if we consider this equation, that is the momentum equation rho u du dx is equal to minus dp dx and then if we non dimensionalize we essentially see that for creating order one change in acceleration you need order Mach number square change in pressure. Also you can show it in a different manner. Let us decompose the pressure this non dimensional pressured as now as the as a background pressure P 0 x theta plus fluctuating pressure P dynamic pressure P 1 x t. Now we assume that let us say that if P 0 is order one let us say that P 0 this is an order one quantity and this is an order Mach number square quantity.

Now, if this is an order Mach number order one quantity, then this will be essentially we can write this as minus dp 0 cap dx minus dp 1 cap dx. So, we will clearly see that on the left hand side we do not have any order 1 quantity. So, then this essentially become 0. However, then the left hand side we have an order Mach number square quantity right.

So, for that essentially then this becomes the full thing that is gamma Mach number square plus times rho cap U cap du x U cap dx. So, this is it.

Therefore, we see that gradient of P cap 0 that is a background pressure is essentially 0 or P 0 is a function of time only, if this not a function of space. So, essentially we call this P 0 rho R T as a thermodynamic pressure and P 1 x t as a dynamic pressure. So, that is the isobaric assumption. So, as a result in for subsonic combustion for all practical cases we our momentum equation is essentially gets very much simplified, because your main thing that is the gradient of pressure that is very small for all subsonic combustion problems and in both in non flemings flame as well as flemings flame we will assume that the pressure to be essentially constant under survive is mentioned. Of course, in certain special cases in a gas turbine combustor or in a after burner or in a rocket engine or in you can have something called thermo acoustic pressure oxidations and then this P 1 fluctuates very heavily.

So, that is a different condition, but other in other cases we will have a small pressure drop and that is small pressure drop will be neglected. Of course, you remember that in a we will show that related in a scramjet instead of a pressure drop you have a pressure rise, and that pressure rise can be large because now it is not a order of Mach number or Mach number square not very large depending on the situation that, but this is that those are high Mach number flows. So, remember that this is only for this isobaric assumption that is a pressure is constant inside the inside a combusting flow is only true for subsonic conditions, so essentially combustion is like characterized by strong change in temperature, but very small change in pressure.

So, it is a essentially a constant pressure process this flow is at constant pressure, but not at constant temperature. So, that is up to this class and later we will go into derive simplified forms of the different equations especially the energy equation because as we see that the momentum equation was very much simplified in this cases for at least for simple flames, but of course, if you want to solve the flow inside a combustor you need to go complete c f t you need to solve the complete momentum equation and in to a you to take the different terms for arising from the pressure small pressure gradients we need to account for those also we need to account for the retain density variations you need to account for the viscous forces and of course, you need to account for the flow acceleration.

But for the simplified cases that we will consider here at least in the beginning of this in the next few courses we will consider pressure to be constant, but of course, temperature will be strongly changing and using this constant pressure or the isobaric assumption we will derive simplified forms of the energy equations and the species equations. And we can see that how will it can be coupled to simplify the total state of governing equations.

Thank you very much.