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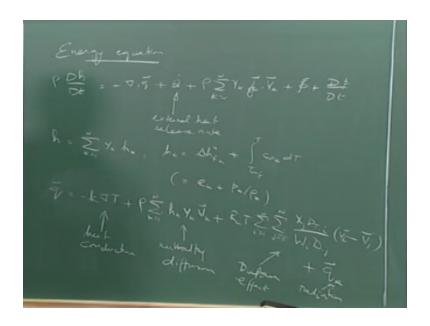
National Programme on Technology Enhanced Learning

COMBUSTION

Lecture 19 Energy Equation

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We were looking at the energy equation so here we rewrite this again where we now look at term by term so this is the this is essentially the inertial term of enthalpy flux right and so the enthalpy is now of the mixture and so H is now written as Σ Y K HK where HK is now the specific enthalpy of species k which can in turn be written as the standard heat of formation of that species time plus the sensible enthalpy okay this is a specific sensible enthalpy of species k.

And temperature is an unknown that is sitting on top of this integral here as a upper bound of course if you want to rewrite this equation in terms of internal energy instead of enthalpy you

could derive this from noting that you can write this as e k + PK developed by ρ K for this HK and proceed from there now let us look at the second term it is the first term on the right hand side here which is the Q vector which is the heat flux vector so the heat flux vector is essentially coming from like from the sides of a particular point in this inter domain and the first contributor is the conductive heat flux which is which is given by the Fourier law so we are assuming a fluid that would satisfy the Fourier heat conduction k is the thermal conductivity of the mixture okay.

So when you now have a mixture of lot of species we have to ask what is this k so similar to the question that we asked about μ may behave a similar question on k as well this is basically transport properties of mixtures which is something that we will have to go back to kinetic theory or molecular level to deduce we will not do this now I will just put it out put out an expression in a website this is coming from the fact that you have diffusive component of enthalpy flux in a into the mixture averaged convection right.

So this takes care of the mixed or average so this will actually conduct the enthalpy of the mixture at the mixture average velocity but in addition to that the species is also taking with it enthalpy of itself at the diffusion velocity this is what this represents which was sort of left out previously, so you have a negative sign here that will take care of the fact that if you now take it to the left hand side that would add up on the actual enthalpy that the state that is taken by the species this is a term that is the counterpart of the so net effect that we saw in multi component diffusion.

This is called the dufor effect as you can see you have the thermal diffusion coefficient DTI /Dij showing up Dij is the familiar binary diffusion coefficient and we had noticed the diffusion coefficient earlier as well in the Dufor effect there we were looking at a concert a temperature gradient contributing to a concentration gradient here it is the molecular diffusion velocities disparity the disparity between the molecular diffusion velocities is what is actually contributing to a heat flux okay.

So it is opposite of what the sweat effect describes but by a similar process or at the molecular level again QR is a general term that is been written out to take into account radiant of heat flux

alright but you should now be able to expand this taking into account things like shape factors and emissivity's versus absorptive and all those things for the surfaces as well as gases that are involved in a volumetric or surface manner and so on the day with a t to the power 4 dependence putting this defense law and all those things.

So if you if you want to drink bring in radiation into account there we are Q.is an external heat will is rate this is a volumetric heat release rate these are this is this is actually having this units like rats per meter square so you are looking at actually a heat flux over here but this is more like a vats per meter cubed because you are looking at volumetric heat release that is within the domain.

So this is typically coming from things like if you now have a very complicated geometry of something like a electrical wire or let us say nuclear rods or something of that sort that is giving rise to heat that is outside of the fluid but you want to now keep that within your domain because it is too complicated for you to negotiate the fluid within these parts but you want to just kind of say on a wall on a spatial distribution basis the per unit volume heat release rate would be so and so if you want to just plug that in.

This is not the chemical heat release rate okay the chemistry is part of the fluid mechanics it is not external this is external okay the chemistry is part of the fluid mechanics sitting here in the Δ HF not k there is the standard heat of formation of species k if you now take that into account and then add it up weighted by the individual mass fractions of species each species then you now get the summation for the standard heats of formation that tells you how much heat is actually released by taking in the heat of formation of the reactants and releasing the heats of formation of the products all right.

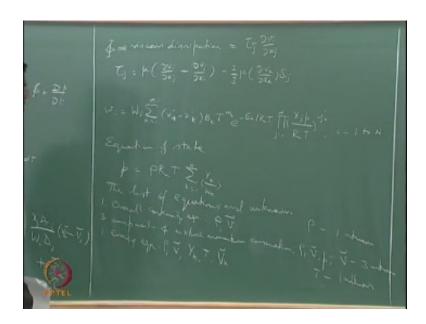
So that is that is already taken into account in the H it is embedded there it is not external this is coming from the fact that recall this equation is a thermal energy equation you could write out the total energy equation by writing an equation for these for conserved conserving the stagnation enthalpy right the stagnation enthalpy would have the static enthalpy plus the velocity squared by 2 right and you get this you now take a dot product of the momentum equation with

these the flow velocity which is flow means mixture mass average velocity of the mixture then you get what is called as a mechanical energy equation you subtract the mechanical energy equation from the total energy equation to get the thermal energy equation.

Well you did that in that equation you had a body force per unit mass term showing up alright and the body force got dotted with the mixture averaged velocity alright but each species is actually getting acted upon by the body for but by a body force that could be unique to that particular species the first place and secondly the work done by the body force is on the species velocity.

A species is trying to move at a particular velocity vk vector okay and then you now have a body force that is acting on it and trying to do a work on this so the work actually should be a dot product of the body force or acting on that species per unit mass okay that is essentially acceleration there okay times these species velocity but we took a dot product of the mixture average velocity.

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So the species velocity is nothing but the mixtures average velocity plus the diffusion velocity and we subtracted only one part of it which is corresponding to the mixed or average velocity but there is still another part that is remaining which is which is based on the diffusion velocity that the reason why we are getting this okay.

And then the this term is the viscous dissipation and we write out the viscous dissipation over here which is again notice this is again using the tensor index the Cartesian tensor index notation over here we are applying the Einstein's summation rule okay or rule of summation will be repeated indices we are having to repeated indices here I and J both of them are repeating all right. So ti j is actually nine terms so it is a second order tensor so it has actually nine components and there we have by tXJ is going to be again a tensor okay.

So this is like a dot product of two tensors alright and so essentially what it means is that you know having nine products that are all getting added up together all right and so we are on a in 3d if we run I going from 1 to 3 and j going from one to three and then we will add up all of that okay. Now how did they get this if you go back and look at your momentum equation you had a $\partial / \partial XJ$ of ∂IJ which gave you the Ith component of moment of your shear force for unit volume okay.

So you had a special derivative of a or your shear stress and we were doubting that with UI or VV I okay, so our work done by the shear stress should have been something like VI ∂ / ∂ x j of ∂ ij that is what we should have had that that is that is actually the work done in the mechanical energy equation okay, here we would have actually had a term that is more like ∂ by ∂ ∂ / ∂ XJ of ∂ IJ V ∂ / ∂ X I of ∂ IJ VI okay.

So here what you are doing is that that is the total energy equation, so the total energy equation you now look for what is the full work that is done by the viscous stresses and then in the mechanical energy equation you now have a term that is dotted by the sheer force with the velocity right and then you subtract that this is what you would you would get you can actually show these things as an exercise and we will we will post these as exercises for you to show okay well while you are doing this course.

And finally of course we now have this DP / DT term that is coming primarily on the right hand side because you are working with a enthalpy conservation if you were to work with an internal energy conservation you will now notice that you have an e k + PK / ρ K you can now plug that in here you now have h that is now summing over you y k e k + σ y k PK / ρ k and then you can now identify.

This term on the right hand side if you know trying to conserve internal energy instead of enthalpy but effectively this is a term that is going to come up primarily because this is the pressure work term essentially okay there is pressure that is acting on a flow that is moving and because the flow is moving you now have a gradient in pressure that is acted upon by velocity that is as if like you now have a pressure that pressure force that the flow is up against and therefore you have a work that is done by that.

And this is typically something that comes up for compressible flows you do not have to worry about it in incompressible flows all right. So this is the energy equation finally we have to close the set of equations that we have had with this expression for WI which is in turn containing your temperature and the concentrations alright because this WI showed up on the right hand side of the species conservation equation.

And that was kind of like an unknown until we try to try to relate it to a set of previously agreed unknowns the perceptive previously agreed unknowns was concentration this is a mole fraction of course what we enumerated first was the mass fraction why I but the moment you actually used the multi-component diffusion equation that equation was on grad X I so we had to now start reckoning X I as our unknowns and therefore we have to have a set of equations that relate xi and yi that is readily available that's an algebraic equation set.

So you now have to reckon excise also as unknowns and show that and see that it shows up here in this expression in addition to the temperature showing up at a couple of places and this is the gayest place where it shows up ok and I would like to remind you of this is the temperature sitting in the denominator of a ratio which is taken which is which is risen to an exponent with a negative sign all right.

So this is a highly which is a high degree of non-linearity here that simply means that as the temperature increases this term will actually increase in a highly nonlinear fashion that means it is not going to rise as rapidly for low temperatures but it is going to go boom with a slight change in temperature beyond a point that depends on e okay, how the e greater this non-linearity or the greater the sensitivity of the action rate to or the production weight in this case for the Ith species to temperature okay.

So higher the e the greater the delay in temperature axis for this thing to go up but the moment it begins to go up it goes to very high values okay so that is the non-linearity that this brings in which makes it very difficult for this set of equations to be solved already we are beginning to look at a fairly ugly set of equations in terms of just being partial differential equations that are nonlinear not necessarily nonlinear primarily because of the convective term.

But there are all other kinds of nonlinearities that we are also beginning to look at in terms of what the multi-component diffusion equation even the flicks law for part of it shows up for you and then you see this non-linearity here this is actually a product okay this π is actually a product of lot of unknowns over here all raised to coefficients that are not one okay anytime you have a power other than one you have a non-linear term and you now have products of those that is making it miserable on top of it you now have a very nonlinear term that that is sitting there. So this is a horrendous problem as far as combustion is concerned.

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• Viscous Dissipation
$$\Phi$$

$$\Phi = \tau_{ij} \frac{\partial v_i}{\partial x_j} \qquad (219)$$

$$\tau_{ij} = \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) - \frac{2}{3} \mu \frac{\partial v_k}{\partial x_k} \delta_{ij} \qquad (220)$$
• Closure
$$w_i = W_i \sum_{k=1}^M \left(\nu''_{ik} - \nu'_{ik}\right) B_k T^m exp\left(-\frac{E_s}{R_u T}\right) \prod_{j=1}^N \left(\frac{X_j p}{R_u T}\right)^{\nu'_{jk}} \quad i = 1 \text{ to N}$$

$$(221)$$

So we with this we can actually complete the set of equations so what were all have we done so far in t his full set of conservation equations well of course I think I just missed one more equation of state equation of state which is $P = \rho$ or UT times σ K = 1 to n YK / Wk this is pretty much the way the mixture molecular weight is defined all right the mixture molecular weight is primarily defined through what is called as Dalton's law of partial pressures right. How did you get the Dalton's law of partial pressures we know from basic definition of density that you simply have to add up the densities of the individual species to get the dense mixture density all right?

And then the Dalton's law of partial pressures is the one that says that if you want to get the pressure of the mixture it is an addition it is a summation of all the partial pressures. So that is essentially the way we can define the mixture mix the molecular weight or in other words we now say that the mixture will also have to obey the perfect gas law just as well as the individuals species and if that would be if that were to be the case its molecular weight should be like this all right in other words you are saying one over.

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• Equation of State
$$P = \rho RT \sum_{k=1}^{N} \left(\frac{Y_k}{W_k} \right) \tag{222}$$

The mixture molecular rate is equal to one over Σ k =one to n YK / WK that is so that is how we are that is how we are doing this, so what did we need these equations right so what we have to look for is what are the unknowns and then what are the corresponding in some sense all these equations are linked to each other they are all simultaneous set of equations you cannot solve each of any of them independent of the other okay.

So you need the entire set and still what we can think of is each of these equations is meant to be like an evolution equation for a one particular unknown it is unfortunately it also involves other unknowns for which we will go in search of other equations which in turn will be evolution equations for some specific unknowns in our mind okay. So this is this is easy for us to actually try to tag equations and unknowns together okay.

So that we can enumerate them together and make sure that we have the same number of unknowns as the number of equations ultimately okay. So the equations the stuff list of equations the list of equations and unknowns one the first thing that we have is an overall continuity equation right. Now this equation involves ρ and VI where VI is the earth component of the mixture the mass average velocity of the mixture okay, this is not the species velocity this is the

or if you want to use a vector notation which is little bit less confusing you could simply say V vector that means you now are looking at three components in 3d for you to for you to have but this only one equation it is merciless equation it just puts all the mass together regardless of which direction in which things are going right.

Therefore three components of velocity the end density all together will have to be tackled in this equation we would now reckon this as something that is an evolution equation for ρ , so that is one unknown okay, we still have three more unknowns to account for so we continue to go in search of equations . So if you're now looking for a vector as an unknown to be solved for you now look for a vector equation the momentum equation is a good equation for us.

So three components of mixed of momentum conservation right, this involves this continues to involve row which has already been enumerated not a problem this involves the V vector all right that is good. So this we think since things could have been nice if it just stopped here but unfortunately involves P which means for you louder now go in search of one more equation at least for p okay and then we will find that that involves T and then I will find that that involves something else and so on right.

So that is how our lives are gave we go in search of more and more goals and then they get you into other problems and so on so that is what lets how combustion is so lively, here what we would like to keep is this equation is meant as an evolution equation for velocity the mixture velocity so this is actually three unknowns right, so all I am asking you to do here is match the number on the left corner to the math two to the right corner we should try to look for that so long as we keep going doing this we should we should hope that finally we will have the same number of unknowns as the number of equations okay.

So we still have one more unknown that we have to write an equation for and let us suppose that we can pick at the energy equation the energy equation does contain p although it is not really an evolution equation for p okay, we will now see that it involves other unknowns, so one energy equation now this involves a lot of new unknowns right, so it involves ρ which is already been it is all new unknown it is an old unknown it involves V vector all right that was sitting in the

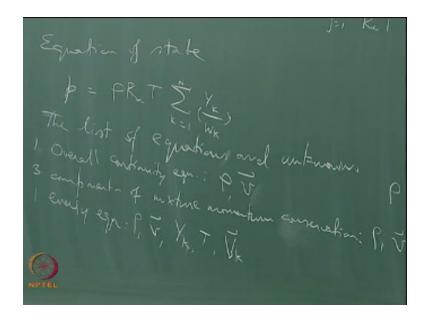
capital D / D D okay in fact the way we can actually find out unknowns is to do it like the way you would do if you are a computer.

So you just can it is like row is it an unknown yes it is unknown d that is not an unknown h is it an unknown h is equal to y k that is unknown, unknown, unknown, unknown, k times n times and then if you keep doing this and then you will find the T's and taken just very bluntly you do not have to be a genius okay, so it is not a very difficult thing to do at all just how to be very patient plotting through equations term by term letter by letter okay and you and then you can find that week V shows up there and yeah we did that right.

So we know we now go from here we now go from here we go we go there YK is an unknown okay and fortunate now for the first time that is n unknowns for you okay that is capital n unknowns and capital n could be 40 50 100 k so that that is one of the nightmares that there is now beginning to show up but anyway we are no hopefully one equation gave it is supposed to be like a template equation for an evolution of something as you now go HK this is fine that is given T sitting there is an unknown and that is what we would now that we'd like to tag this equation as an evolution equation for.

So we have T a enumerated as an unknown already now and then what else is going on so you know how q. q has this K that's supposed to be given well strictly speaking it depends on the mixed refraction, so it is an unknown but we know how to write equations for that relationship between the decay and the mixed refraction okay. So you can always look a lot of things as unknowns and then and then provide equations for each of those ok but let us not do that at this time T is counted HK contains t that is counted YK is counted VK okay that is a pain why is it a pain?

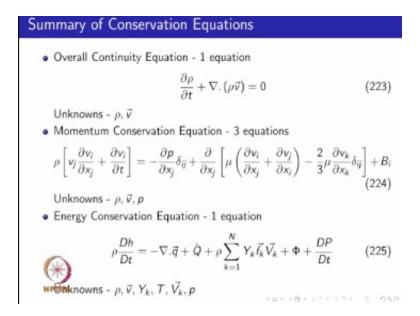
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It is M diffusion velocity vectors that means there is actually three n unknowns in 3d for three components of each and every species diffusion velocity vector right, so that is a lot of fun hostess is proliferating by the minute with the energy equation looks like a big villain here, so we had this that this is okay so we have already counted all these things we are doing fine and then we go back here FK is supposed to be known p is already counted the Phi involves essentially the mixture average velocity that is been counted good okay.

So what are we what are we come across over here it is we will now call look at this as a evolution equation for T which is one unknown but we are grossly under estimating the problem here because we have now to reckon three unknowns here and sorry three n unknowns here and one n unknowns here right.

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So we are short of four n equations, the good news is anytime you are short of a equation for a vector you look for a vector equation because the vector equation will give you three components by itself all right yes, pressure is also there yes p is also there fortunately for us that is been counted okay, so that is not an extra known anymore thank you. So we now are now hunting for four n equations okay, so what is the first equation that we can think about that there is like a set of n equations let us see species conservation equations right.

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So the species conservation equations are n species conservation equations and species conservation equations in one of the species conservation equations contain they contain your YK right, so we had a ∂ V ∂ Y K / ∂ t as the first term unsteady term then we had a convective term which involve the mass average velocity if the mixture V vector small V vector then we had the diffusion velocities of species.

So right we had this right and then we had we had let us say a WK you either write WK here and then count this n equations separately or you now say well I can write plug this expression on the right-hand side of that and note that it has these X and T and so on so I do not have to write separately this expression is just one term one huge term that there can be plugged on the right hand side of that equation without having to count it separately.

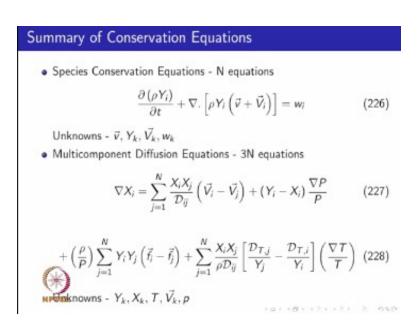
So let us suppose that this is what we have, now I would like to look at this equation as an evolution equation for y k that is n unknowns I want to basically say this n corresponds to an end there just for the just for the purpose of tallying okay every step of the way okay what are we not still done we do not know what is this okay is it all not quite if you were to plug this if you have

to plug this n you now have a xk or an XJ that is not the same as y YK unless all the molecular weights are assumed to be the same it is not necessarily the case in general right.

So we also have to now reckon the mole fractions of individual species as unknowns all right okay, so we are now still stuck with chasing for n unknowns okay fortunately for us when you are now looking for a evolution equation for this is the vector and we can now look for a vector equation so three and multi component diffusion equations right in 3d of course right, so this involves this involves YK or right xk or write a capital v k all right then we also had pt thinks all those things that have been counted so far right.

So what it basically does for you unless I am missing something more to just point out if you if you if you have the equation right in front of you can go back to see if anything more is involved in here a small s K vector is supposed to be given it is not considered an unknown and similarly other parameters like.

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DIJ and DTI and so on or consider to be given okay, so here I would like to look at this equation as a evolution equation for not really an evolution it is not evolving things but it is basically a

constitutive relationship for capital v k vector that gives you 3 n unknowns pn unknowns, so you have a three and here on the three and there that is okay.

But what are we still missing we are we have still have to count xk write as n unknowns therefore there must be one set of n equations and relationships between YK and xk involving all the molecular weights okay, did we did we close the set maybe not you just go back we have taken care of row we have taken care of t we still have to worry about p we started out with thinking that we will go through the energy equation in search of p but we tagged it to t.

So this is this is now 4 X K this is n unknowns, so we were counting 5 + 5 + n over here and then now you say 5 + 4n okay and then this is 5 + 5 n this is 6 + 5 n, so we are essentially looking at a total set of 5 n plus six unknowns and we have 5 n + six equations to solve for okay this is a question that is asked for me in my PhD qualifying exam okay.

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Summary of Conservation Equations

• Relations between
$$Y_k$$
 and X_k - N equations

$$X_i = \frac{Y_i/W_i}{\sum_{i=1}^N Y_i/W_i} \qquad (229)$$
• Equation of State - 1 equation

$$P = \rho RT \sum_{k=1}^N \left(\frac{Y_k}{W_k}\right) \qquad (230)$$
• (5N+6) unknowns and equations!

What is the total number of equations and unknowns are yeah in combustion okay and list them that means you have to let us both the equations and are the unknowns okay so you just have to muck this up 5n + 6 that is like a magic answer hmm, and then start scratching it I am sorry start counting thinking okay but this is a click this is they actually a decent way to think about this like each and every equation is supposed to do the job of solving for you and unknown okay.

But it involves other equation other unknowns that you will now go and search off for with it for other equations okay, and then we have to now close the set this is essentially the idea what we are here 5n + 6 what does that mean? Even if you took a modest number 4n as like 20 you are in trouble we are now looking at 106 equations and unknowns that we need to solve for and these are ugly looking equations okay, if you were to take a more realistic situation of 40 species okay you know again a 206 equations you see you see the problem right.

So there are people who do these things it is as if like I am NOT making this up okay, so you look at the pages of things like combustion and flame or proceedings of the combustion institute or combustion Science and Technology combustion theory and modeling any of these things you

will find people who are actually doing these kinds of things so it is not just to boast that that we have lot set it is something like a burden that we have to go through right.

Then we have to think about is it is it required for you to actually keep cranking these numbers all the time for each and every term in each of these equations because you have the large number of equations and so on there are many ways by which you can handle these things like for example if you know we are thinking about a typical equation keep in mind we have a convective term you have a diffusion term and they in a reaction term right.

So these three terms have their own typical time scales the pins you do not have to necessarily evaluate each of these terms in each and every equation all the time that means you are just cranking up numbers right the idea is the reaction time scales are typically very small things are happening pretty fast you are looking at fast chemical reactions in the reaction zone right so you now have fast reactions that are happening the timescales for these reactions is so short that the flow is hardly moving when you are now trying to evolve how the composition is changing because of the chemical reactions.

So for all you care you could actually freeze the flow okay an advance it over large time step and during this time you can now do your chemical calculations alone you do not have to worry about the flow field it is like frozen right so that means you go back to an expression that looks like this and then say this is DCI over DT like an Eau de all right at a particular place and then you now are given a concentration set of for all the species here at the particular point if I now take a small time step here how will I advance to the next small time little later to change the concentrations based on a just a time integration of this set of equations okay.

Given that the temperature is whatever it is right there all right and then keep doing this for quite some time until the composition has significantly changed and then start moving this round mixing it with other places and convicting it and so on, then you know bring in the other parts of your the other terms of your equations. So this is like a multi time scale approach that allows you to what should I say reduce the amount of calculation that is required you see, so you can now look at this like a separate package that will that will keep on cranking but before you actually

crank the fluid mechanics right so the bees you do not have to worry about taking small timescales to resolve this and the fluid mechanics simultaneously the fluid the fluid is not going to take these species too far from where they are as they are changing because of chemical reactions.

So you can freeze the flow during this time so you can take these kinds of approaches to simplify your life but life is certainly complicated if you now look at the full combustion problem why would what we would do from now on now on is we now have actually looked at the full combustion problem we have post the combustion problem okay for any situation this set of equations is not valid for any situation of combustion problems what we will try to do is it possible for us to simplify this under certain conditions.

So we will now we are now reached like a summit and then we will keep going downhill to make it easier for easier for our lives and then we will now start looking at specific problems like let us say a pre-mixed flame or a diffusion flame and so on within a simplified framework that is handle able from a theoretical point of view rather than having to rush to a computer every time to do anything right, so this is this is the way the rest of the course is going to go from here this is like the starting point from here we will now go simplifying things. Thank you.

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