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Lecture 17
Multi-Component Diffusion Equation

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So we need to actually look at this multi-component diffusion equation that means we need to look for something that is a substitute for Fick's law that is applicable only to a binary mixture so we need to know what to do for a truly multi-component system so let us let us now just write out the equation.

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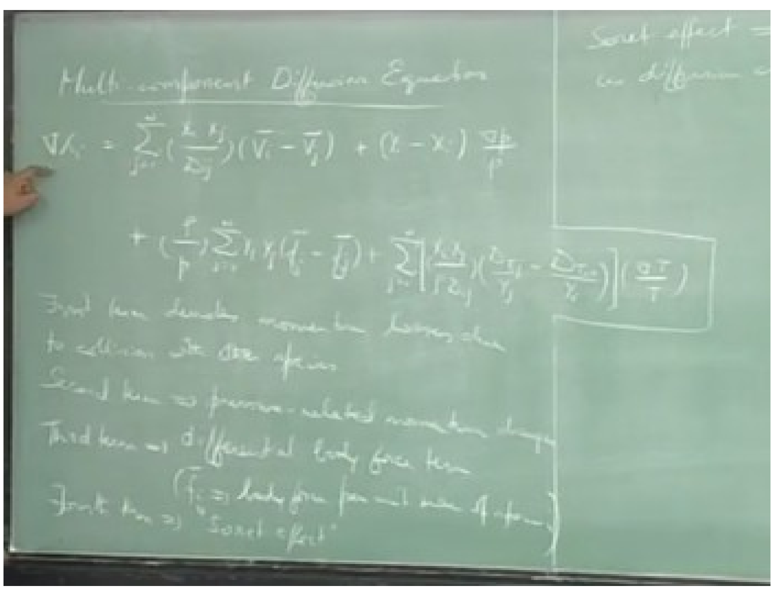

It is going to go like ∇ Xi = Σj = 1 to n, Xi Xj / Dij Vi vector - Vj vector + Yi –Xi / ∇p / p + ρ / pΣ j = 1 to n Yi Yj times fi Vector – fj vector + Σ j= 1 to n Xi Xj/ ρ Dij times Dt, j – Dt, i / Yj I am sorry this ought to be like this Yj – Dt, i/Yi times ∇t / t so probably use a okay so does that look like Fick's law at all could Fick's so what does it mean and I do not understand I just wanted to go from two species to three species what life get so difficult I guess when you get married you going from one person to two percent life gets very difficult right.

So this is not terribly bad now let us be big here we can think a little bit more rationally than there right so if I were to basically say can I reduce this to Fick's law situation that means if I now say my N = 2 but I get Fick's law back where I or would I not obviously not this is obviously a monster when compared to what we were talking about previously but if I now said I have only two species would Fick's law be hidden in it could you see could you see fig peeping out of anywhere here remotely can you recognize him right.

Yes we can first of all what the word how did we get this okay well huh we I just pull it out of my hat and that is it you just try to take it from me like it did like God given the answer is pretty much like we said that Fick's law has to be from a molecular level basis instead of a continuum basis we can derive this from a kinetic theory consideration but this is actually considering a lot more than fig ditch empirically deduce for his set of conditions okay so we now are looking at about four different things out of which Fick's law is contained only in this term first okay.

Because I can I tell that because I started out looking for a relationship between the mass diffusion velocity of species I to its concentration ∇okay and if I were to looking if I were to look for a mass diffusion velocity related to concentration ∇ I really wanted to look for a concentration ∇ in terms of mass fraction rather than mole fraction but this is what I have okay so any hope of getting Fick's law is from here because that is what is first of all containing the mass diffusion velocity of species I.

Unfortunately it is also containing the mass diffusion velocity of species J which is not = I okay if it were = i then you would have a 0 here Vi - Vr okay so if you had two species this is actually a convoluted expression for the ∇ the ∇ of mole fraction of one of the species in terms of concentration sorry mass fraction mass diffusion velocities of the two species that are involved so if I can if I can now write this for ∇Xa okay and then ∇ Xb what I am actually looking for is Va in expression for Va and an expression for Vb.

So now have two equations again I can now solve for one of them and then the problem is I will now have ∇X_a and ∇X_b which I did not have before but then try to convert that from XA to Ya and so on okay so you start doing that then you can try to get that so whatever we were looking for is only in one corner of what the full picture is so what is what is going on so the first term first term denotes momentum losses due to collision of collision due to collision with other species.

This is the this is the mechanism that is actually in play in Fick's law as well okay and the second term so you now start looking at what are these different terms these are pressured related momentum changes pressure related momentum changes the third term we now have to explain what is f is body force per unit mass of species I is fi vector.

Fj vector is body force per unit mass of species J right so what is body force per unit mass it is kind of like acceleration okay, so in a gravitational field this would simply be like G except you would be wondering why would G be different for species I then species J the answer is no gravitational field mostly are not going to be looking at here this is more like things like electric fields magnetic fields and soon okay.

So we are dependent upon whether your species that you are looking at is neutral or positively charged negatively charged you are going to have different body forces on different species right therefore this term is primarily coming from a differential body forces okay keep that in mind I am highlighting this because as we are looking at the second term there is a pressure related momentum changes go back and look at that you had a $\nabla p / p$ that basically says that this is driven by a pressure ∇ that means a pressure ∇ causes a concentration ∇ is what you are essentially saying.

But also keep in mind there is a coefficient $Y_i - X_i$ I oaky we will be looking for situations where these are not important so for example here if the pressure ∇ is not there then there is no contribution of that to concentration ∇ okay or you could be looking for situation when $Y_i = X_i$ when would that be we talked about it right that is when all the species are having the same molecular weights of course is a somewhat like a fictitious situation but for ease of analysis we could assume that if you want to consider pressure ∇ otherwise okay.

But you do not want so we should be looking for when these different terms are important and so on so one of the things here is you could get rid of this term if you do not have any body force to consider on any species in the first place that means fi and fj already 80 or if you have to keep body forces for some other consideration get rid of here you now take advantage of the fact that this is actually differential body forces therefore if the same body force is acting on this on all species then do not worry about it like gravity.

You want to take gravity into account okay but gravity is going to act on all of them okay then equity there you do not worry about this term so this is what is going to happen so this is a differential body force term differential body force term and so here for example fi vector is body force per unit mass of species i same holds for j and you are looking at the difference between the two this is a vector difference keep that in mind okay this is a vector equation on the whole.

So this actually has three components in three dimensions yeah and so it actually caters to your need we are looking for aVi vector to be modeled in terms of concentration ∇ that it does that this is a vector equation right away and finally the fourth term full term is called slow rate effect this refers to thermal diffusion okay.

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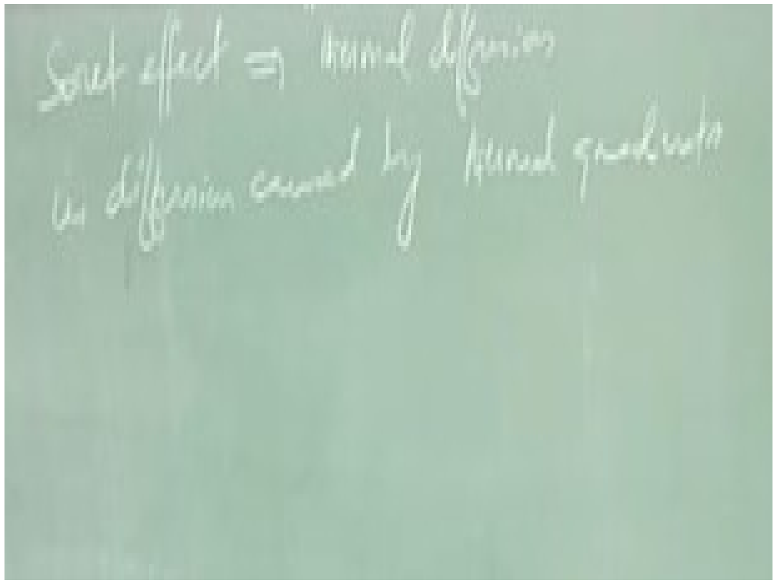

So sore it effect thermal diffusion that is at here is a diffusion caused by thermal ∇ so okay when we are looking at the energy balance we will look at the opposite possibility that is if you now have species of different concentrations that could give rise to your heat flux all right that and that we will we will recall we will now we will call that as a do for effect and this is a Seurat effect these are named after these scientists.

So here this is again all these things all these things are deduced from molecular level considerations like in kinetic theory and what you would find is that if you had temperature ∇ as you can see here if you had a temperature ∇ that contributes to a concentration ∇ okay so that is the effect that you are looking at okay and we would mot derive this as I said we just state this okay.

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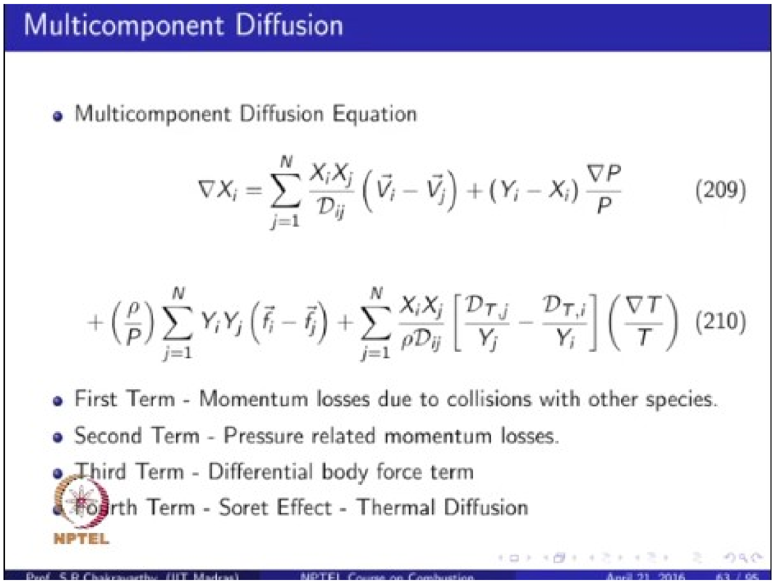

Now it can be shown it can be shown that that means you show a.

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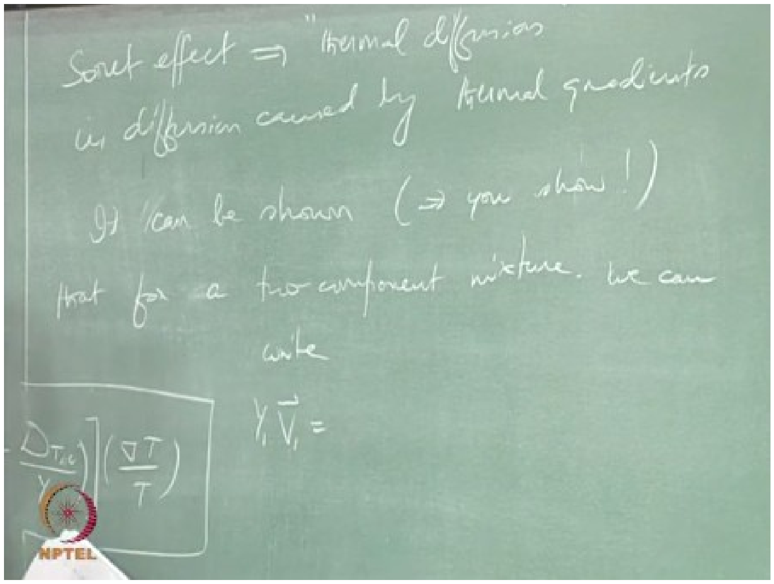

Shown that for a two component mixture for a two component mixture we can write we can write Y_1 V_1 vector is equal to V_{12} ∇ Y_1 - Y_1 Y_2 / X_1 X_2 times Y_1 - X_1 times ∇ p / p - Y_1 Y_2 / X_1 X_2 the whole squared ρ / p f1 vector - f2 vector + DT, 1 / ρ D12 ∇T / T now DT, 1 or DT, i in general refers to what is called a thermal diffusion coefficient okay so DT, i refers to a thermal diffusion coefficient that that just shows up here or here okay.

Now typically you can also you can always see that okay let us just look at the units of these this equation here you are looking at ∇ of X does not have any units it is a mass it is a mole fraction okay so a ∇ will have like one over meteor kind of thing so you are looking at 1 over length kind of units ∇ T / T also has same units okay because they need the T units get cancelled and then you have only ∇ of something non dimensional.

Therefore and of course you look at this x and y they do not have any units okay so what matters for you is D/ road DTI or DTj / ρ Dij is what should be dimensionless okay I am sorry yeah that is right that is right so this is this is having the same units as this that means everything else should be dimensionless and since x and y is do not have any dimensions DT i/ ρ Dj that is how typically you would compare things so DT i / ρ Dij is small alright typically.

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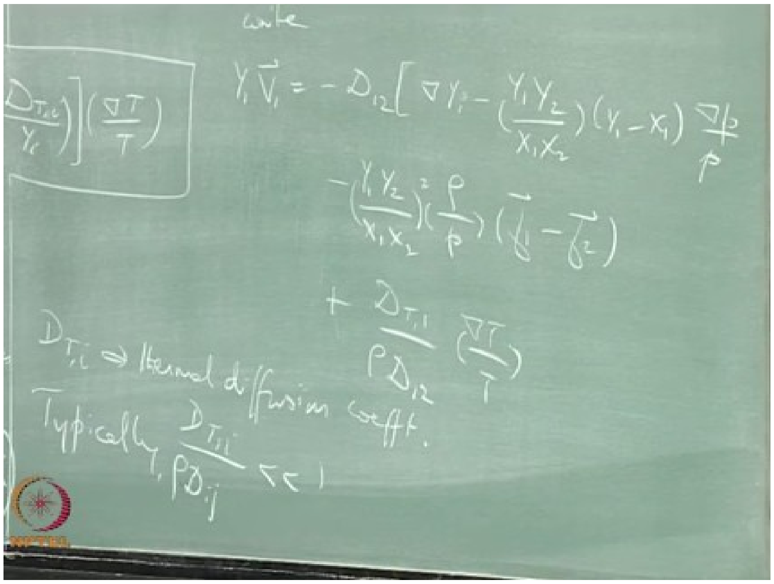

So now they are just to get an idea of what is going on if you were to just look at the Dij alone it is the highest for gases okay that means gases can diffuse very fast alright but lower for liquids and then still lower for solids you can be thinking about solids also going through a molecular level diffusion all right like in like an alloys and so on but that is a very slow process I mean compared to what happens in gases so this is fairly high.

So the if you compare the they are like orders of magnitude different as it is again as you will see but if you now compare the thermal diffusion coefficient with the ρ of the mixture times Dij for a pair of gases then this is obviously not for a pair of gases this is for one particular gas alright whereas the Dij is a binary diffusion coefficient it is pair of gases okay the other thing that I would like to point out is when you now have a multi-component diffusion equation and you are looking at the same the same process that was there in Fick’s law showing up in this term.

You are still retaining the binary diffusion coefficient and then summing over all other species than what you are talking about okay we do not have to explicitly say that J is n= I, I over here because that would contribute your 0 okay, so you could just sum over but essentially we are looking at the interaction of all other species one at a time with species I okay so it is as if you now have a multi component mixture and you are looking at what is the concentration ∇ contribution due to mixing for a particular species it is coming from this species interacting with all other species individually in mixing with all other species individually as pairs of the species.

And each of those other species individually okay and as I said Dij = Dji for any pair i and j and so it is like species I is mixing with any speech any of the species J other species J all other species J are equally mixing with species I in turn a it is kind of like if you now have a group of people and then you now let a bad guy in this bad guy actually interacts with each of the each of the guys in this group so every person in this group is equally responsible for entertaining this guy and contaminating the group you see.

So this is this is what is going on we are now still looking at a binary interaction and a corrective effect of the binary interaction over here all right this is a little bit indirect because we would like to think of a diffusion coefficient that is a function of only one species at a time we do not want this pairs of species business because you think about a thermal conductivity or a specific heat or something of that sort we can easily think of those as being properties of only one particular species right.

But its diffusion coefficient we have to think about a pair of species at a time that makes things complicated we will try to work around it by some kind of assumptions and simplifications a little later but at the moment I have to point out that is how the process is mixing always involves minimum of two species at a time and we always can look at them as a process that involves two species at a time even in a bunk bunch of species together right so that is a reason why the same binary diffusion coefficient that we saw for a fixed law shows up here and that is what exactly what it is here as well okay.

Now we can as I was talking about we were trying to get rid of some of these terms so that we can now begin to see the Fick’s law come up right and I also told you can we apply this can I can we apply this to your binary mixture and that is this result you can see that this is little bit different from that that means some simplification has been made okay it is been made so that we actually have Y1 V1 vector which is the diffusion mass flux that is what Fick's law was looking for okay.

To get you something in terms of concentration ∇ in terms of mass fraction concentrate mass fraction ∇ right so we this is this is already read it rewritten in this form that we want now we have to look for what are the conditions under which you can make simplifications and retrieve Fick's law out of here.

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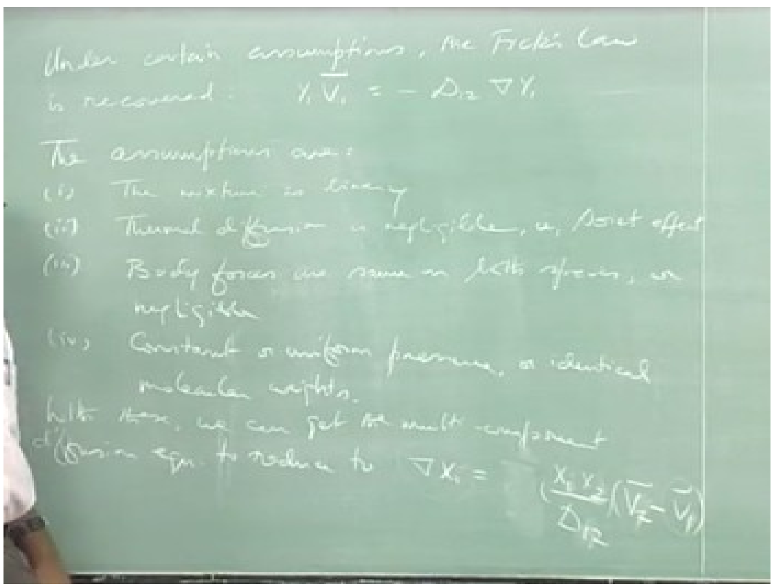

So under certain assumptions and that is what we are see now certain assumptions under certain assumptions the Fick's law is recovered okay that is to say you can say Y1 V1 vector is equal to – D12 ∇ Yi did we see this well you all you have to do is put in a ρ on either side if you now put in a ρ Y1 becomes P 1 P 1 B 1vector becomes j1 vector and that is = - ρ1 D12 ∇ Y1 that is exactly what we had before okay so this is this is pretty much the same as what we saw for the Fick's law.

So the assumptions are the assumptions or one the mixture is binary of course we are looking at applying this to a binary mixture in the first place the thermal diffusion is negligible let us see so ret effect that is in whatever we do you know in our class we will always be pretty much assuming that the soy defects effect is negligible because DTI / ρ Dij is much less than 1 we would not worry about it for most of the moisture conditions okay three body forces body forces or same on both species or negligible you have you have two choices of making assumptions okay.

So again you can assume that the body force is the same even if they are not negligible or if you have to get rid of it you have to make an assumption that it is negligible the question basically is you know for example if you are now looking at buoyancy effects that means you cannot get rid of body force okay buoyancy effects in flames and it is very typical and under gravitational conditions.

So the reason why you see these candles flames looking elongated upwards is because we are in Earth's gravity if you now go to a zero gravity environment you would not see this kind of a shape right so if you want to actually think about that effect not exactly that affect me there are some things that go associated with that shape for as far as the heat transfer back and all those things is concerned so from a quantitative point of view gravity does affect not just the shape of the flame but lots of other interesting parameters.

So you might want to keep gravity but fortunately for us the gravity would affect different species to the same extent so that is fine so it does not affect this equation it shows up in the mixture momentum equation okay so keep it there you do not have to worry about it here constant pressure or constant, constant or uniform pressure constant or uniform pressure or identical molecular weights right either of them will sell if you had a grad P that is 0 that is okay proximately or if Yi is approximately = Xi that means both the molecular weights approximately the same then that would work as well.

Now how good is this assumption or either in any of these assumptions the answer is not terribly bad although it is not strictly valid in it and the most conditions you can think about so many times when you are looking at assumptions you have to ask yourself is it a reasonable assumption to make or is it completely unreasonable just to make our life simpler all right the answer is you will find we will go through this quite carefully under will we will note that under typically low mach number conditions all right.

And most combustion processes that we commonly encounter right from candle flames Bunsen burner onwards kitchen gas stoves onwards to even highly turbulent flames and furnaces gas turbine combustors and power plants and all those things are all fairly low Rockets they are all fairly low Mach number hello any ideas hello point two, point three is low it is not even that high hey typically it is point 1 or less many times it is like point 01 all right.

Now if you really think about what I am talking about okay now are these kinds of temperatures that we are looking at the speed of sound is so high so you are looking at something like close the temperatures close to the adiabatic flame temperature the speed of sound is like of the order of 1000 meters per second right and point 1 times that is going to be like 100 meters per second that is going to be very fast it is not slow really strictly speaking but the Mach number is low because of high temperatures involved you see and typically we are looking at fairly low subsonic conditions for most of these.

And what we will show is under those conditions it is okay we will show that the pressure actually becomes constant more or less all right, so this is not this is not terrible or if you now look at molecular weights if you think about molecular weights between for example nitrogen and oxygen there is not hardly any difference okay so like looking in between 28 and 32 carbon monoxide is what about right 16 + 12 is again 28 okay carbon dioxide is a little bit of a high on the higher side but methane could be like about 14 water is like 18.

So they are all in the same ball park for from for most part so it is not a terrible assumption under most conditions your nutrition too much worry too much about the molecular weights being too desperate they are not for move for most punt conditions so for analysis purposes it may be okay to make this assumption but not a lot of times for example looking at propulsion you have like the specific impulse or something like that is going as X quite out of T divided by molecular weight.

And it is in the denominator so if you now have a small change in the molecular weight let us say from if it changes from let us say 20 sorry 30 to 20 or like 28 to 18 it makes a difference it makes a significant difference in your is p calculations and so on and people die for getting that kind of increase in ISPs from there so you got to be careful on the application and you might be able to get away with assuming equal molecular weights for the purpose of getting rid of this term or for the mind of binary mixture this term.

So then with these we can we can get the multi component diffusion equation to reduce to ∇ Xi = Σ j= 1 to n Xi X /Dij times Vj vector – Vi vector right that is what we can get it too so if you want to now make sure that this is a binary mixture make this i is 1 and so j = 1 to 2 we can now make this X1, Xj D1 and so on and be one what we are interested if you now go back and look at look at this and this are there okay do not have to worry too much about Dij because j goes from 1 to 2 and j is unequal = 1 so this is just going to be only one term right.

So we do not have to worry about a summation you can you can j is going to take one we value of 2 and therefore you can get rid of this and then start putting your j is 2 for you can now have a j2 D12 and V V2 the problem that I am talking about is you now have V2 X2 and X1 as distractions from this expression is he did not they do not and then of course you have X1 here you wanted a ∇ Y1 but this is an expression for ∇ X1okay.

So you know how to convert wise to axis k there is a relationship between x and y for each species which involves all other species that unfortunately okay but this is a binary mixture therefore you should be possible to for you to figure that out and also you have to eliminate V2 the B2 you will have to consider the next equation and so on keep in mind in a binary mixture X1 + X2 is = 1 and Y1 + Y2 is = 1 you shake you should use with additional equations and then you should now simplify this to something like this that is an exercise as well for you to do right okay I think we will stop here for the day we start too late.

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