Indian Institute of Technology Madras

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National Programme on Technology Enhanced Learning

COMBUSTION

Lecture 15
Mass and Molar Diffusion, Fick's Law

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So we have been looking at these different models of combining chemical and thermal processes like the fixed mass reactors of constant pressure and constant volume and then we looked at the open flow systems of well stirred reactor and plug flow reactor the question is what can we do with these okay so many times we can actually use these to solve complicated problems in more simplistic manner but something that is quite interesting is you could also actually use combinations of these models to set up like a network that deals with a more complicated system so one thing is to take one system and try to simplify it into one of these but another way is to actually put a bunch of these together in a network that will mimic a more complicated system.

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So the model reactors can be used in a network so for example so we have let us say a gas turbine take a gas turbine combustor so we know that for example you now have a gas turbine outer casing that goes like this and then you now have a feeling lab that comes in and then you now have a swirled so you have an atomizer here you have a spoiler and then you have a liner and so you have some swell cup and so on so you now have the primary air that goes through this the secondary air goes like this and this is fuel this is air and then you have this line you are having these holes for secondary I have to come in so you now have a finally commercial zone here and a secondary combustion zone here so this is of actually different phyla ratios.

So you now have like a close to stoichiometric mixture over here and then you now have some air that is coming in further into this and you now have a more fueling condition of combustion there and then you have a further situation of dilution because you now have to have the turbine blades withstand the temperature at the outlet so you need to have the turbine entry temperature reached at a particular and not higher than that therefore you have these called dilution holes right so this is this is like a flow that is a diluted flow diluted not just in not in terms of air but also in terms of temperature that means you are relatively cooling this gas so this is the primary a combustion zone secondary combustion zone.

And this is the dilution zone so how do you deal with this in a they are actually highly complicated system in terms of the fluid mechanics that is involved here the chemistry the combustion all those things are the multi-phase flow although all the stuff that happens here t is a highly complicated situation so how do you try to use the simplified model reactors that we have had like the double the well stir this is obviously a open flow system.

So you have to actually choose something like the W I saw and the PFR that we have seen before so what you can actually think about is you now treat the primary combustion zone as a WS r1 and then what happens is so you now have a fuel line and a airline that are feeding into these so you now have a Inlet from the air and the fuel right.

And the exhaust of the WSR 1 gets into the gets into another WSR right that can be used to simulate the secondary combustion zone and you now have this airline can keep going you now take additional air in here and then the output of that gets into well it depends on whether you want to treat this as a PFR or so on but typically you do not have too much combustion going on and you are now at the tail end of the combustor.

So you could actually more easily treat this as a PFR and you can even keep track of how things evolve in space because pf4 allows you to do that in a one-dimensional manner right so you could you could try to model this is a PFR with additional air and then you now have this coming out right in case you are thinking of having a additional fuel that is participating in the secondary combustion because if you now have incomplete combustion in the primary zone.

And it is not just the combustion products of the primary zone that feeds into the secondary zone but additional fuel you could have this as well just to just to be sure that you are using all the field that is in there in the inside the combustor so you see that this is now like a network of these, these model reactors in tandem one after the other and also using what the output of one has an input of the other and so on and taking air from a airline and feel from the fuel line for these different parts differently and then finally you now get these are the two inputs and that is the output there is a there are temperatures for these.

So that means you have a enthalpy for this in there fucker spawning Lee you will get the enthalpy for that and so on so something of this sort can be done so I would like to conclude the section on these model reactors which combine chemical and thermal processes without getting too much into flow details except for the little detail that we did for the PFR and without getting into any mixing at all and, justify trying to avoid mixing and deal with quite complicated situations in a simplistic manner but then we cannot avoid mixing completely.

So we have to step into getting intermixing as we go along so we will let us now start doing the real combustion real combustion now involves you to be dealing with convection diffusion and reaction all three together so we have so far been looking at chemical reactions and we did not really do too much of convection or flow we would not do that much but we will have to ultimately get into some amount of mixing that we need to look at that is what we would want to do.

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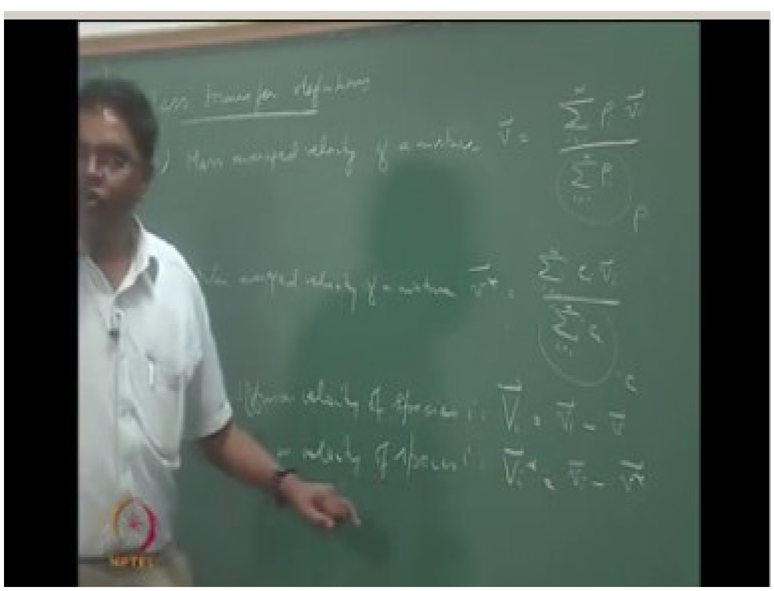

So we want to now look at some mass transfer definitions okay this is actually continuing from the set of definitions we had on mass concentration of species and molar concentration of species and mass fractions and molar fractions so he be most fractions we have made these definitions earlier on but now we have to actually get into a conceptual idea here so the, the first definition that I would like to make is again we will have two parts one is the mass average velocity of the mixture let us suppose you use develop the symbol V vector small V vector for velocity of the mixture this would be defined as i =1 to n σ ϱ I VI vector / σ i = 1 to n ϱ I what σ i =1 to n ro I do you remember from past that is just the density of the mixture itself okay.

The density of the mixture itself is nothing but the sum of all the individual densities of species because the density s nothing but mass per unit volume so per unit volume of a mixture let's suppose that we have air around us and then air is a mixture of let us say nitrogen oxygen and a few other things in trace so you just pick a unit volume of this then you start counting the mass the amount of mass of nitrogen amount of mass of auction and so on and in this amount the mass of nitrogen per unit volume is the density of nitrogen the mass of oxygen per unit volume is density of oxygen.

And so on you know add up all the masks that is there in that that is the mass of all the all the species there per unit volume is the density of the mixture so it's simply adding up all these so this is not this is nothing but Rho so you are now begin to see that if you do not have a subscript right it now may it now belongs to the mixture if it has a subscript then it belongs to a species all right first of all and then how does it work the density is summation of all the individual densities but the velocity is like an average it is a mass weighted average why is it why am I saying n as waited because this is actually a mass average velocity right so I could have I could have simply said this is mass of individual species times its velocity per unit volume divided by mass of individual species per unit volume.

So I could have had like per unit volume on both sides so you got the density from the mass so it is essentially a mass weighted average or velocity of the mixture what does this mean is if you now have a mixture of gases what we are try and then each of these each of these species is actually trying to go with its own velocity alright and since I am showing my thumbs that that is to actually indicate the direction the pains you now have the a species a goes this way a species B goes this way and so on at this particular location and time right out of this we are now trying to picture how the mixture is going to go on the whole without worrying about what the individual species are doing so how do you deduce how this mixture is going to go as a whole we now try to average the velocities weighted by their m as that means if you have a very small amount of mass of a particular species it does not really count too much for the mixtures velocity let us say you have a very small amount of mass going very fast okay you are still going to have the mixture on the whole going slower.

Because lots of other things which are present in greater abundance are going slower right so as a mixture it is not going to go just as fast as this very small component right so this is what we are saying we could have also done this instead of having a mass average what else could we have done mol moles right so you can use moles so the molar average velocity mixture we now call this small least our vector that is given by σ i =1to n CI VI vector / i =σ, i= 1 to n CI.

Of course this is also the same as C which is the concentration of the mixture the molar concentration of the mixture because it is also going through the same kind of arithmetic which is just summing over all the number of moles of all the species together per unit volume all right so what is happening here is the mixture actually is a mixture traveling at a velocity V or is it traveling at a velocity V Star though they are not same okay the see eyes.

And the row eyes are not exactly the same how are they related there is a molecular weight coming into picture okay so they would actually be the same if your molecular weights of all the species with the same but that is that xenon necessarily true you could have hydrogen on one hand which is a very low molecular weight when compared to let us say butane okay a carbon dioxide all these things have much higher molecular weights so these are not necessarily the same the question then is what is exactly the mixture doing is it going at this speed or is it that speed it depends on what you want how you how you want to deduce the mixture speed.

So the mixture speed is not an absolute quantity it is the species velocity that is that is more absolute the mixture velocity depends on the we want to evaluate the mixed velocity right it is kind of like saying or in a democracy you have a lot of people who have to get together to vote and select the leader okay so if they now select the president in one country or the prime minister in the other country who is bigger the president of the Prime Minister no it does not matter the people of the ones that are the most important that is what the democracy is all about right so here it is a species velocity that is really that the loot how you want to actually deduce some extra velocity is up to you right this is now going to be very important the next step that we make right.

So the next thing that we want to do is a we now define amass diffusion velocity of species I species I okay now this is actually for a individual species and the way we want to define this is capital the AI vector is equal to small vector minus small V vector and let me just complete the next step be and then we will talk about this molar diffusion velocity of species I is now capital the I star is equal to VI - V Star vector.

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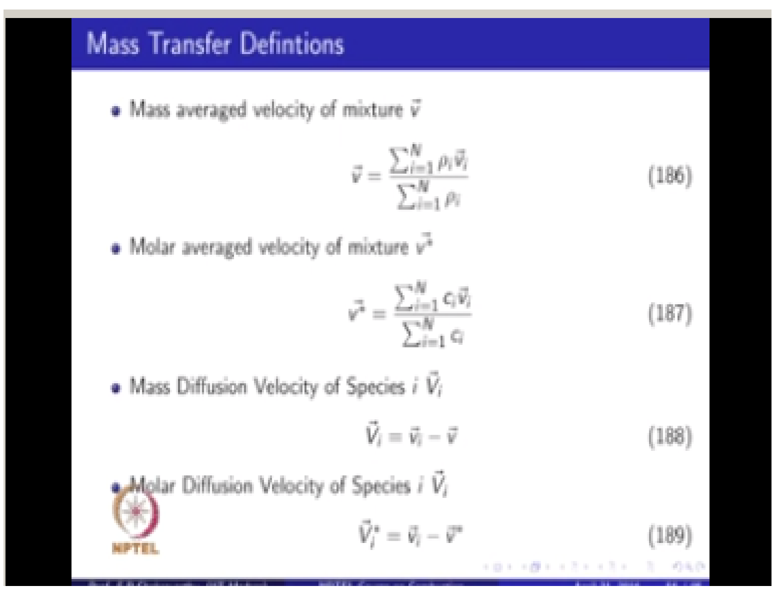

You see here v is are the same because they are absolute they are always there as they are okay depending upon whether you are subtracting the mass average velocity of the mixture or the molar average velocity of the mixture you now get apparent velocities of the individual species which are capital v or capital vstar and why do we say apparent what is it going on it is like saying this is where we have to really listen okay it is like saying you now have a mixture let a air okay right there in the picture okay so you are now into your combustor you now peeping into your combustor.

And then you finding a lot of species going hither and thither right you want to now try to deal with this like a mixture so you now choose to pick a mixed a velocity that is defined either this way or that way all right and then you now want to tag this mixture velocity to the mixture in reality all species are going this way in that way then you got a mixture velocity out of this that is going that is saying that the mixture is going like this.

And then you go along with it that means these velocities are in the mixed a fixed coordinate system we are essentially transforming our coordinates if you are in the lab fixed coordinate system where you had your combustor running and then you saw your species going this way and that way and you could deduce a mixed a velocity for it as whatever it is for the mixture that is going in whichever way you want it is all in the lab fixed coordinate system.

But now you decide to travel with the mixture when you are traveling with the mixture at the speed that you have determined for the mixture in a certain way right you begin to see that the species are going this way and that way it is not all going like this okay because you are going along okay it is going like that is even going backwards right because you subtracted out the mixture velocity right so you can now this is vector addition this vector algebra okay so you are looking at vectors so from your mixtures fixed coordinate system it looks like as if the mixture is stationary right that is very good because forget about the combustor forget about aerospace engineering and all those things we will now take a box okay keep the mixture on our desk table.

So I am going to go anywhere let the mixture mix right because the mixture is not going anywhere we are going with an extra anyway right so while we are going in the mixture we are now in a mixed-effects coordinate system so the next two is now on the table you do not need to you do not need to go anywhere so whatever you are going to be looking at for the species velocity if the mixture were not moving is what you are going to see with this or this right and that is how we would have actually tried to make experiments to try to find out what else is the mixture is doing other than going I am sorry what else is the species doing other than going with the rest of the mixture if you now have air in this room I suppose we do okay.

And it is a mixture is a mixture of nitrogen and oxygen predominantly and then you want to now try to start looking at what the oxygen molecule is doing okay we do not really bothered about things at the molecular level because we want to stick to a continuum framework so the particular point if you want to look at what is oxygen doing what is oxygen species velocity that is actually a bunch of molecules millions of oxygen molecules at this particular point collectively what are they doing when compared to the rest of the mixture rest of the mixture is mostly nitrogen so you know ask what is the nitrogen doing okay we will find that most of them new moves to the time in what we are thinking about the auction is pretty much going to do the same thing as what the nitrogen is going to do.

Because it is all completely mixed when it is completely mixed it is now acting as if it wants Fiji's air then the paints the species are going to do the same thing that means they are just going to go as one single species which is the mixture right so what do we understand if a species is going to do something other than going with the rest of the mixture then it is not completely mixed right and to qualify what it does other than go with the rest of the mixture is what you have these velocities for right so this is a and this is very important this is fundamental to anything that you do with mixing yeah so this is this is leaked now mixed your fixed coordinate system right this is lab fixed coordinate system.

So in general let us make this point very clear in general Smalley and small v star k and capital VI and capital VI star or different or different for species in a mixture with just similar molecular weight so okay and this is going to come to haunt us after some time yeah so sometimes you will find combustion a scientists analysts are making these seemingly reckless assumptions like equal money molecular weights for all species what is a big deal I mean continued even deal with more species that are of two different mall he hates the answer is yeah but we have lots of other equations to solve.

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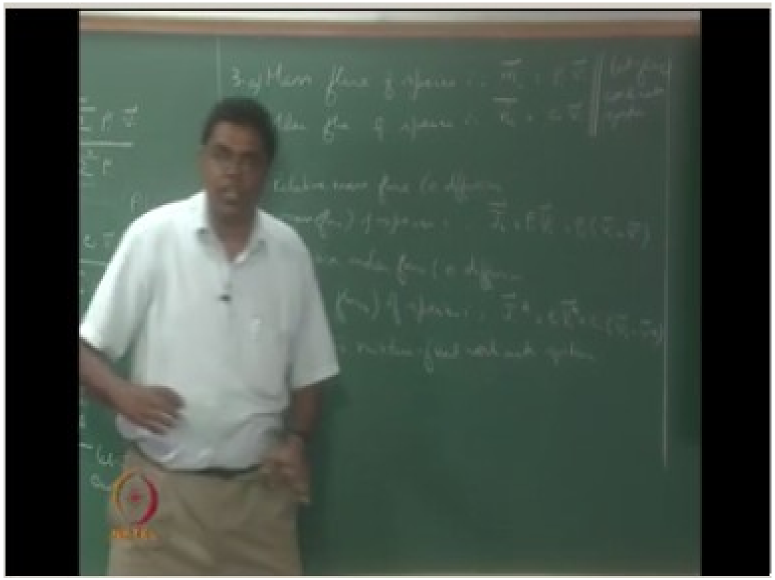

Now we can we get some reprieve here we will find okay so what we do with this we can now define mass fluxes where we are now stepping up our approach towards something particular so of course we know that mass flux of species I there is m.vector I =ϱ I VI okay and of course we have an A and B molar flux of species I let us call this dot vector =C I VI does it VI is a absolute so this is in the lab fixed coordinate system right something that we are familiar with mass flux is nothing but density times velocity a similarly molar flux is nothing but concentration times velocity all right.

Then we should now be able to write for a relative mass flux relative mass flux or diffusion mass flux diffusion mass flux of species I is vector is equal ϱI capital VI which is ϱ I VI - V right and be go through the same thing replace the word mass by molar and then we will see how the symbols change a little bit let have molar flux or diffusion molar flux of species I how does the change star is equal to ϱ R I am sorry from CI capital VI stall vector that is equal to C I VI vector minus V Star vector right and

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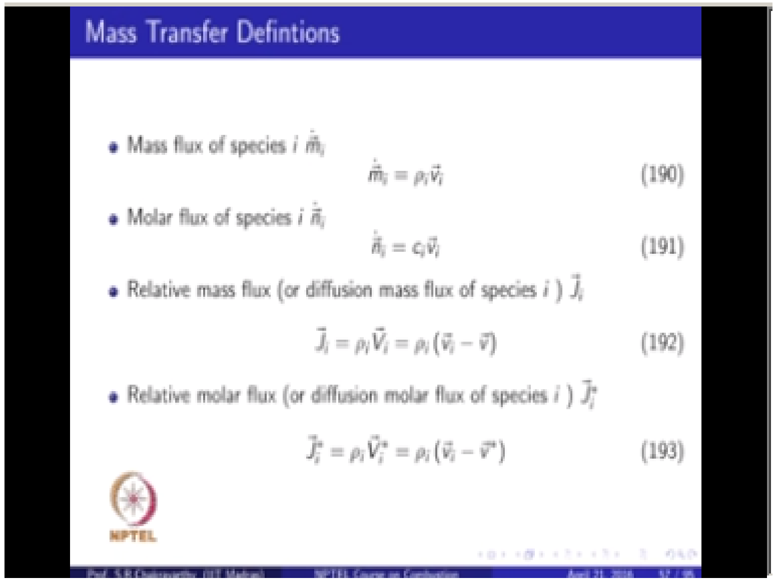

Obviously this is in the mixture fixed coordinate system right that is no mixture fixed coordinate system what are we done the first thing that we have done is for the first time in our lives we have used the word diffusion okay welcome to the confusion the moment you have diffusion you are going to get into trouble okay and that is what that is what we will we will see for from now on and so obviously things get more interesting exciting and stuff right whatever we have been doing so far it is been boring and then what you are saying is if you are now thinking about math walks let us actually think about in a mixed a fixed coordinate system right.

So in a mixture fixed coordinate system if I were to move with the mixture right what is the mass flux of my species that is going here and there it is all not going in together in one direction because I am going along then I am subtracting that, so you could now also have some mass flux or molar flux depending upon how you want to look at it go backwards forwards either this way that way and soon right so why are we interested in this flux where could not we have just talked with velocities right that is because that is how fixed law comes about okay so we now have to have what is called as flicks law?

We are now ready to look at flicks law at all sick around 1858 stated that the a star is equal to minus C D A B gradient XA for a binary mixture of species A and B the plural of species of species okay so we say species we are talking about individual species I you know talk about two species A and B all right okay we got it now it is very likely that fake exactly did not say it in a mathematical way but we are now geared up to state flicks law in a mathematical way right and because we are now come from a mass averaged and molar average velocity.

All the way to a relative molar diff you molar flux or diffusion molar flux J I star for a particular species right what it basically what did he say? he found that the relative molar flux or the diffusion molar flux of a particular species is directly proportional to its mole fracas little portion its concentration gradient one would you have a concentration gradient if you now had a variation in the concentration in space.

Okay that means you have more of it here more of a particular species here less if a particular species there then you now have a variation and a spatial variation would mean that you now have a good Ian and that is what is actually driving the species to come from thereto here right that simply means that you do not have a mixture in which all the species are uniformly mixed if you had all the species uniformly mixed like we think air is around us at the moment.

Okay then we would not have any concentration gradients of oxygen here versus here versus here and so you do not have any gradients that the means oxygen does not rush this way while nitrogen is rushing somewhere else or the mixture is going somewhere else all right of course then the auction rushing this way counts for the mixture going somewhere anyway okay so in a lab fixed coordinate system it will look like the oxygen is going like that but it does not do that other yeah besides nitrogen going somewhere else they are all going together.

Because we do not have any concentration gradients that means the mixing is perfect it is only when you do not have a perfect mixing right you have to worry about concentration gradients and when you have concentration gradients you now have these species go from a region of higher concentration to a region of lower concentration until the concentration gradient vanishes and then the species does not go anywhere it is all living happily ever after right so it was kind of like Robin Hood okay take the money from here from the rich give it to the poor until all of us are living happily ever after okay that is what transport processes always do okay so the DA b is a binary diffusion coefficient that appears as a constant, constant of proportionality between the diffusion molar flux.

And the concentration gradient right and this is a transport property this is amass transport property correspondingly the momentum transport property is your kinematic viscosity and the energy transport property is your thermal diffusivity all of actually have the same units guess is meter square per second right and what do they do their job is to take mass of a particular species from a place where it is no and put it in a place where it is less take momentum from a place where it is more that's what viscosity does okay so momentum from a place where it is more and put it in a place where it is less take heat from a place where it is more and put it where it is less that is heat conduction.

So that is what conduction means so this is like transport phenomena out of which we are essentially looking at only one part which is the species mixing in a mixture right we have to look at something a little bit more carefully we are now saying it is a binary mixture that means we are now looking at a mixture which has only two species how does it matter and how does it work out for does it does not make sense we are doing combustion and do we deal with mixtures that have only two species what combustion means you have to have reactions right so for reactions to happen you need to have two reactants yeah sure so we have two and then they will mix but what about products if two reactants are required to form a third product you do not have a binary mixture anymore easy.

So we are out in fiches not good enough for us right away unless you had like one of them as a reactant the other one is the product yeah that's like a recombination reaction you now had a molecule that that just let us say you it was subjected to heat from the flame let us say okay and then it decided to reorganize itself and become another species okay like a like a bunch of atoms in one corner of the molecule started getting excited dissociate and then go around and then form and then go back and course you know find that you now have radicals and all the stuff right because it is all got dissociated.

And so on so it is on the binary species is something that we do not really come across typically but you could if you want to simplify your situation you say a equals B is my global reaction I will deal with Molly two species and so okay you could do that but flick do not really have that much of a complication in his mind okay he was only looking at a isothermal may be non reactive okay mixture of two liquids as a matter of fact is what he was doing right so whereas it is an incompressible situation and because I as I said j star is a is a is a mixture fixed coordinate system you do not have to worry about a mixture in motion in a lab fixed coordinate system you could think about a mixture that is right in front of you sitting there mixing as you speak or observe okay.

And then you can come up with this law and therefore the sea is a concentration of the mixture just like in an incompressible flow you say the density is constant they say the concentration is constant for the mixture as a whole can be pulled out of the gradient and then you now have amole fraction gradient rather than a concentration gradient right so this is the simplistic sitting in which thick really came up with this law okay and you could of course so we have a of course we could we could write in terms of in terms of diffusion mass flux let us say we are not chemists so we are not used to dealing with things in terms of molar flux where we are more used to things in mass flux.

So let us say diffusion mass flux J a =-ϱ it is the same be as before you now have a mass fraction variant rather than a mole fraction gradient and I density instead of concentration in the constant for the coefficient J a star becomes J a vector right so what is DAB, DAB is the binary diffusion coefficient binary diffusion coefficient for a power of species A and B.

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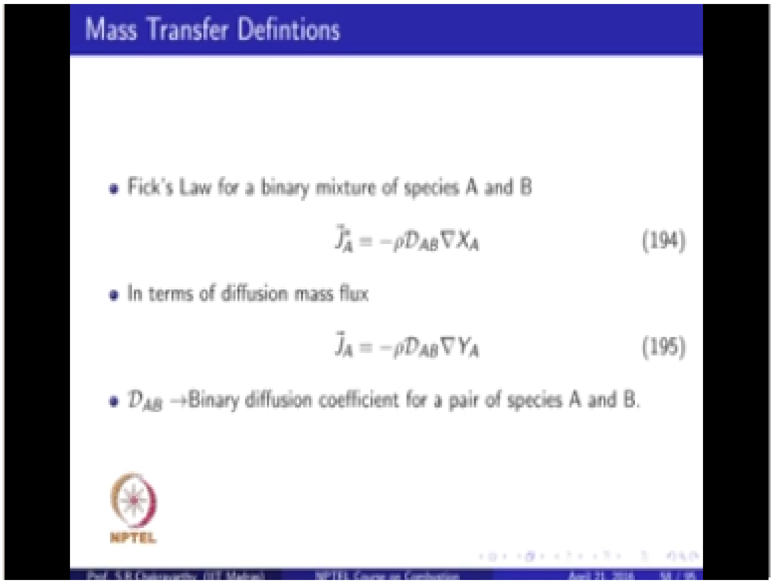

So the binary diffusion coefficient is actually defined always regardless of how many species are there in you mixture okay you can still think about a binary diffusion coefficient that is defined for a pair of species in that mixture you are now beginning to think a little bit more okay is it possible fours to apply this to a mixture which has more than two species may be okay when what would be a BB yes you can still use the DAV that is a binary diffusion coefficient for a power of species said so it is always valid for a pair of species but what if I have a mixture of B and a instead of A and B well I have a DBA that is different from DAV ah it like a 10-0 or something like that no right so DBA b is equal to DBA that is because we are now in a mixed a fixed coordinate system right.

So if and this is very important because we have a mixture fixed coordinate system effectively what it means is if species a is mixing into species B then correspondingly species B is mixing it a species say just as well so it was like saying if you now have hydrogen and oxygen they think that hydrogen is a much lighter gas when compared to oxygen's o you know how a bunch of hydrogen go over here and then my bunch of auction over here in a box with a diaphragm in the middle and then you now have like we have very magic wand that makes this there are from disappeared at T =0 there stop looking at this at t >0 okay you expect that all the hydrogen is going to rush into the oxygen.

The oxygen just sitting like that huh and then you say all hydrogen was the one that did the job of mixing auction did not do that i am thing on the action is going to say yes are you mixing right it is got it looks just as well into the high rhythm s high rhythm mixes into oxygen it is from the Augustine's point if you hire the genes do is done you see this is very, very important okay.

In a in a in a binary mixture there is nothing like this species is mixing more than that species right why are you doing this why do we need the flicks law the fixed law states that the nerve diffusion flux gay or the mass diffusion flux are directly proportional to a concentration gradient in terms of it in a mole fraction gradient or a mass fraction why did we need it what did we need fake why are we talking about right what are we achieving any guesses if you are you think a little bit more.

Okay I told you that these are these are there is a transport process and then there was there are responses a mass transport Gators correspondingly momentum transport in energy transport and you now had viscosity and conductivity come up in those as transport properties what do they connect okay so if this is like a proportionality constant between a mass flux and a concentration gradient what was the viscosity a proposal was viscosity proportionality constant of anything it was a proportionality constant that was relating shear stress to velocity gradient okay keep in mind velocity is a vector a gradient of velocity could be a tensor and therefore you have additional problem in momentum transport of dealing with a gradient of a velocity that means your shear stress could be a tensor.

And so on okay but whereas here this is a vector gradient of a scalar that is a vector okay but then again get back to energy transport things are back to normal we are now looking at the thermal conductivity showing up as a proportionality constant of heat flow there is relating heat flux to a temperature gradient right temperature is a scalar good tough temperature is a vector heat flux is a vector right so what is going on we are always trying to relate some of these quantities like diffusion mass flux or shear stress or heat flux to gradient spatial gradients in concentration or velocity or temperature these are all quantities that I can measure I can stick a probe.

And get my concentration velocity or temperature these are things that are actually showing up in my equations I have a control volume there is a heat that is coming in from the surface or mass that is coming in across the surface control surface and so on and I do not know how would I know I can only measure concentrations in two places to find out it is more than that then it is that you have a mass flux I now measure temperature at two places if this is more than that I know have a heat flux right so in our system of equations we would like to keep the unknowns as essentially our primitive variables right but you now have these heat fluxes mass fluxes and shear stress coming in as extra items along the control surface like for example shear stress is essentially a surface force is coming through a surface force.

Okay to drive the momentum heat flux by conduction is trying to influence an enthalpy change right similarly mass flux by diffusion is going to now change your mass balance you continue the equation right and we would like to relate these two thinks that we want to keep us keep us our primary unknowns and we do not want to deal with any additional notes so this equation and it is like the momentum transport.

And energy transport or constitutive relationships that connect a secondary unknown to a primary unknown now plug this in an equation which treats X a as it is unknown you are safe you are not reckoning additional unknowns you see so this is very important to us unfortunately we will be groping to see how to deal with this for a truly multi-component system where you have a mixture of more than two species next class you.

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