Heat Transfer And Combustion in Multiphase Systems
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Lecture 19
Interface Behaviour

So, in the last class, we, for the interfacial heat and mass transfer, we included the effect of surface tension and the disjoining pressure. And we found out the equations for continuity momentum as well as the energy okay.

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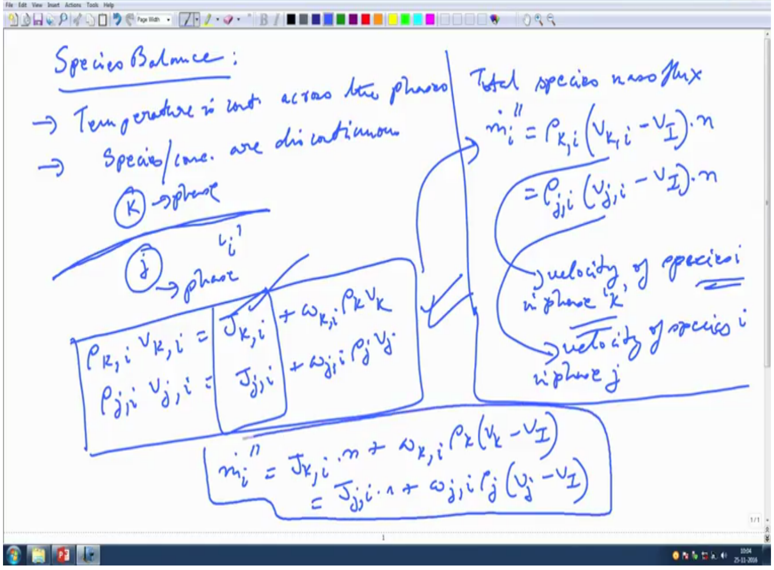

Species Balance:

→ Temperature is cont. across the phases

→ Species/conc. are discontinuous

(K) → phase

i

(j) → phase

$$\rho_{k,i} v_{k,i} = J_{k,i} + \omega_{k,i}\rho_k v_k$$

$$\rho_{j,i} v_{j,i} = J_{j,i} + \omega_{j,i}\rho_j v_j$$

Total species mass flux

$$\dot{m}_i'' = \rho_{k,i}(v_{k,i} - v_I)\cdot n$$

$$= \rho_{j,i}(v_{j,i} - v_I)\cdot n$$

velocity of species i in phase 'k'

velocity of species i in phase j

$$\dot{m}_i'' = J_{k,i}\cdot n + \omega_{k,i}\rho_k(v_k - v_I)$$

$$= J_{j,i}\cdot n + \omega_{j,i}\rho_j(v_j - v_I)$$

In this class we are going to do the species balance okay before we move on to specialized topics. Now in the species balance unlike temperature, the temperature is continuous across an interface right temperature is continuous, right across the phases or across the interface correct, right.

But species our concentrations are basically discontinuous, right, okay. So, okay so, general interface if we consider a general interface between two phases say phase k and j right, okay. And there is a mass flux and in phase a, this is phase k and phase j. Now the species that we are considering is i, okay.

So, there is a migration of species i or mass flux of species i, between these two phases right, okay. So, k and j are not the species, these are the two phases okay, i is basically the species, okay. Now the total species mass flux which is basically m dot i okay is basically, it will be given as and we will come across each and every one of them in details okay.

I will see what each of these terms exactly means ji okay. Now this v ki what you see over here is basically nothing but the velocity of species i okay in phase k, right, okay. Similarly this ji means the velocity of species i in phase j right, okay. Like k being here it was one phase, this is the other phase okay.

So, similarly over here you have basically two velocities that we have defined okay. Now these velocities are further defined like this Rho ki v ki = jk i + got it, okay. On the other hand this you guys already know from your previous lecture's, got it, okay. So, this is the velocity that has got a diffusion component obviously okay that is the diffusive flux as you know, ji is always the diffusive flux, right.

So, the velocity of species i in phase k is represented in this particular fashion okay. Now if you substitute these relationships okay back in the main governing equation which is over there okay. You get your m dot i double Prime Jki dot n omega ki Rho k vk - vi = Jji, got it, okay. So, that is now the species flux of the ith species remember always this is for the ith species that we have determined this flux term okay.

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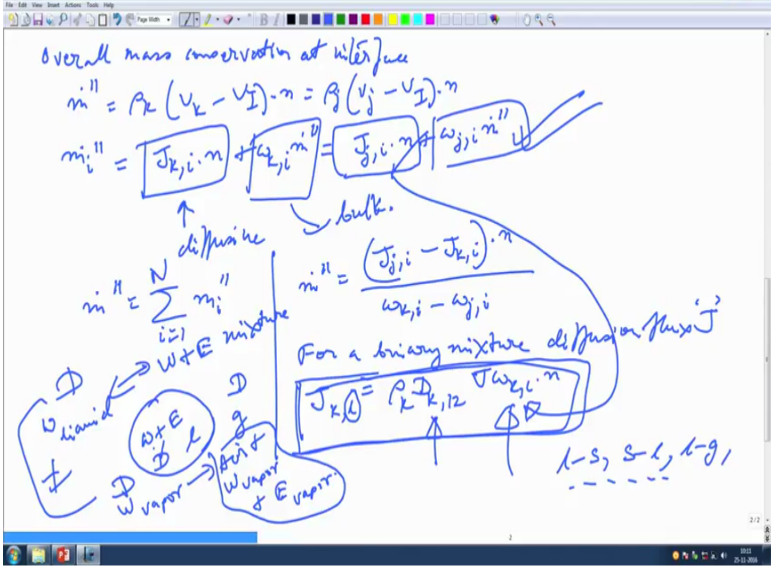

Overall mass conservation at interface

$$\dot{m}'' = \rho_k (v_k - v_I)\cdot n = \rho_j (v_j - v_I)\cdot n$$

$$\dot{m}_i'' = \boxed{J_{k,i}\cdot n} + \boxed{\omega_{k,i}\dot{m}''} = \boxed{J_{j,i}\cdot n} + \boxed{\omega_{j,i}\dot{m}''}$$

diffusive

bulk.

$$\dot{m}'' = \sum_{i=1}^{N} \dot{m}_i''$$

$$\dot{m}'' = \frac{(J_{j,i} - J_{k,i})\cdot n}{\omega_{k,i} - \omega_{j,i}}$$

W+E mixture

For a binary mixture diffusion flux 'J'

$$\boxed{J_{k,1} = \rho_k D_{k,12} \nabla \omega_{k,i}\cdot n}$$

Now the overall mass conservation at interface this we already did in the last class if you recall was basically this, right. This we already did in the last class itself right, okay. And based on this your m dot I double prime now can be written as jki this is the diffusion term + omega ki m dot double prime right, okay = J ji dot n +s omega ji m dot double prime, right, okay.

So, you can understand, so, there is a diffusive component, there is a bulk component correct. So, this is basically nothing but the diffusive component and this is more like the bulk component, right, okay. Because if you look at this carefully from the previous equation how we have actually written it, is that if you look at this particular term say for example here this is nothing but the diffusion.

This is the diffusion of species i through the phase k okay or through the phase j correct, okay. While on the other hand this is nothing but the bulk velocity with which phase k is actually moving or phase j is actually moving and as it is moving it is carrying with it the mass fraction okay of whatever that species is right, okay.

So, it basically has got two components bulk and the diffusion right. So, that should be kind of clear to everyone. So, this is always the case, so, you have a diffusion of species and then you have a bulk of a bulk movement right, okay. So, diffusion happens because of the diffusion because of the diffusion coefficient right, okay.

And bulk happens because it is about migration okay of one fluid into another okay. And as you know m dot double prime is equal to summation of m dot i double prime i to whatever n that you have, got it, right, okay. So, if the species flux is not specified okay the total mass flux will be okay, got it. Now for a binary mixture or a binary mixture this diffusion flux J okay you know how to represent it for any particular mixture okay.

This is basically represented as something like a Rho k D k12 want to bring the two components this is basically nothing but the concentration gradient, look at it later, okay. So this is a very standard fickian diffusion kind of a model right where this is the diffusion term and this is the concentration gradient, right.

So, you can understand in one case this component was transported by the bulk movement right. This is actually transported by the concentration gradient. So, this term is very much like your heat conduction kind of them your Fourier heat conduction, There is a concentration gradient instead of D there you have k right.

And so, there is a transfer of heat here instead of transfer of heat you have a transfer of mass right. You have a transfer of species in this particular case okay. Now the binary mixture can be in the presence of any of the phases. So, for example here we wrote it in terms of some arbitrary phase okay.

It can also have it in terms of say liquid-solid, solid-liquid then liquid-gas it can be with respect to any two combination of phase’s right, okay. So, it does not necessarily mean; so, it is basically whichever phase it is presenting, it is the diffusion in that particular phase, right, okay. Say for example you take the example of say a droplet because droplet is something that we will cover immediately after in a short while.

So, the droplet say it is a binary droplet, let us assume for it is a binary droplet okay. By binary it means let us say a water and ethanol is actually present in this particular droplet, water mixed with ethanol right. And this droplet is actually evaporating; this is the phase boundary site. So, this is the liquid phase, this is the gas phase correct.

And what happens in the gas phase both water and ethanol actually evaporates and get mixed in the gas phase right. So, that; so, the diffusion of water in ethanol in the liquid phase when you are talking about this binary diffusivity right, when you are talking about this right, that coefficient that D will be very different from the D that you have here, got it.

So, the evaporation of water vapour in air right is very different from the diffusion of water vapour in air is very different from the diffusion of liquid water in a water ethanol mixture got it, okay. So, liquid water obviously, this water liquid okay is actually diffusing in our water plus ethanol mixture right, okay.

So, it has got a certain value of diffusivity okay. On the other hand water vapour in the vapour phase is diffusing okay say in air plus water vapour plus ethanol vapour right, okay. So, it is diffusing in all three of this okay. So the diffusion coefficient is D and this D are very different. They are not equal to each other okay, that is what we mean right.

So, that you can easily imagine that in a gas the diffusion is pretty fast whereas in a liquid the diffusion would be very slow got it, okay. So, but the idea was to give that it happens mass transfer of species transport across the interface happens principally because of diffusion and this, right, individual diffusion and the mass transfer that is happening okay between the two phases okay.

So, this actually governs the evaporation from here you can imagine things like evaporation condensation and things like that, right, okay.
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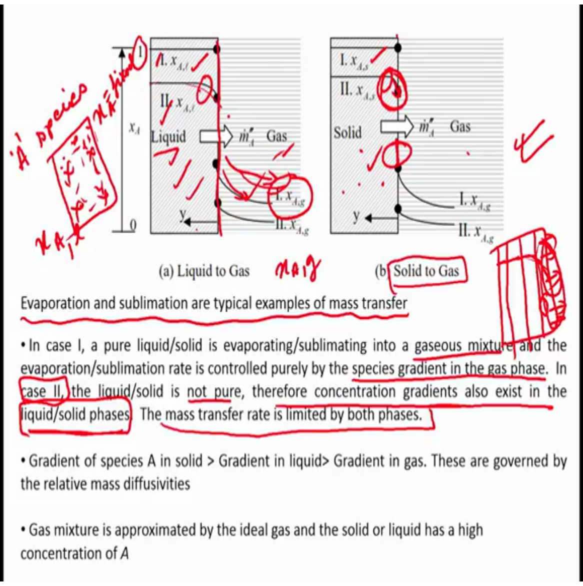

(a) Liquid to Gas (b) Solid to Gas

Evaporation and sublimation are typical examples of mass transfer

- In case I, a pure liquid/solid is evaporating/sublimating into a gaseous mixture and the evaporation/sublimation rate is controlled purely by the species gradient in the gas phase. In case II, the liquid/solid is not pure, therefore concentration gradients also exist in the liquid/solid phases. The mass transfer rate is limited by both phases.
- Gradient of species A in solid > Gradient in liquid> Gradient in gas. These are governed by the relative mass diffusivities
- Gas mixture is approximated by the ideal gas and the solid or liquid has a high concentration of A

So, now let us look at this example that we have over here okay. So, this example can be of various types but let us look at one significant one okay. So here is the example let us take a liquid and a gas okay and the interface is flat okay. So, let us not talk about curvature and any other things the depletion of vapour pressure and stuff like that okay.

So, the liquid for the species here is xA right, A is the name of the species. A is the species that is present both in the liquid phase as well as in the gas phase, got it. So, if we look at this particular thing in details that there is a liquid phase and then there is a gas phase that is that are present okay. What is happening what we are trying to do so this is not a pure liquid this is not a pure gas, right, okay.

So, there is this liquid has got several species, one of those species is A okay. So, when this A the the fraction of A inside this particular species is denoted as xA, x Al, when it is present in a liquid phase. And when it is present in the gas phase it is denoted as x Ag, right, okay. So, this is basically the mass fraction okay of the species A in both the phases okay.

This is direct corollary of the example that we just now saw okay. Now on the other hand this particular figure this is a pure evaporation problem right. This is how things, we have put it you have a saucer filled with water, this is how it actually; will put it right. On the other hand you have this solid to gas interface also sublimation naphthalene if you have seen okay.

So, that is a solid gas media or two phases separated by a sharp interface, this is a liquid gas media separated by a sharp interface okay. So, evaporation and sublimation are typical examples of mass transfer, got it, two cases of mass transfer. Now in case one if you look at, this is one, if you look at case one okay it is a pure liquid or a pure solid which is actually evaporating or sublimating okay into the gaseous mixture okay.

And it is purely controlled by the species gradient in the gas phase right because why it is flat that is because there are no other species present right. There is no other species the value has to be equal to one. If it is a pure liquid say we are if operating pure water this is pure water and that is pure that is atmospheric air right.

So, in the liquid phase you are not going to have any gradient with respect to the water right. Because it is only pure water it will be always one right, no matter what you do it will be always one right. So, here are in on but on the gas phase it need not be one because water vapour is going into air right.

So, air basically has got oxygen, nitrogen and all these things right. So, whatever is only a very small fraction of the air, right. So, once it evaporates you can see that you develop a gradient okay, a species gradient in the gas phase okay. But you do not develop a species gradient in the liquid phase, got it. In both the cases, got it, okay.

So, the concentration gradient also exists in the liquid; in the case of two however in case two that means it is not a pure liquid any more like the example that I gave it may be water mixed with ethanol, water are mixed with something else right, okay. It is not pure okay therefore concentration gradients will also exist in the liquid and the solid phase also here and here you are going to have that concentration gradient right.

Why there will be a concentration dip can you explain that, that is because okay it is basically supplying right, the liquid is actually evaporating or that species is actually is evaporating and going into the gas phase right. So, if it is water, water is getting converted to water vapour, since it is getting converted in to water vapour okay.

There has to be a slope near the interface right otherwise how would it match the flux right. This particular gradient, this particular slope has to match the flux with which the or the amount of water vapour that is actually escaping or the amount of liquid that is getting converted to vapour right.

Like for example in the case of heat transfer what happens, that slope basically gives you how much heat is transferred right q = - k dt by dx things like that right. Here it is basically the mass flow of species A right. So, this is what actually happens and there is a depression of the concentration gradient. Here the concentration is lower, here the concentration is higher. That is because at the interface right were evaporation actually happens right.

In that particular region, if you consider the mass fraction of A is actually lowered it has to be lowered right. If you look at this particular evaporation these things are all interfacial phenomena is not happening from here, here, here, here is always happening from this zone, right. It is not boiling right, so, it is only happening across the interface right.

Since it happens across the interface say initially you had a system say for example okay, where everything was kind of homogeneous right. So, if you ample water from any portion of this mixture it will always give you that xA value and that xA value is some kind of a fixed value, got it, okay. So, that is true that is because that composition is not varying.

But however as soon as you start having evaporation from one of this side right, from this surface what happens is that locally the concentration of water vapour will be lowered, right. That is because some water in that zone is actually escaping. Some water in that zone is escaping into the vapour form. So, if you look at it in a kind of a kind of a discretized fashion right.

If evaporation is happening in this zone right, so, here the concentrations of water vapour will be more or less the same, right. Only in this zone it will start to drop that is because water is getting converted into water vapour locally okay. As a result the other component with whatever that is the other component that with the other species that are present over there okay locally the concentration of this particular guy is getting reduced over here okay.

It is particularly true for example if you have water mixed with some other non volatile solvent right. If you do that you will find that a water vapour concentration at the surface will continuously decay, okay. Similar thing happens in the case of sublimation as well okay because there are two species okay.

Now so, the mass transfer rate is basically limited by both the phases this and this how quickly we can supply it and how quickly we can take it away, right. If it is a diffusion driven phenomena which in most of the cases it is right there is no flow as such right. There is no flow assistance over here okay.

What you will find is that the water, liquid water gets evaporated into water vapour that water vapour is basically transported away from the interface right by diffusion. Because here the slope is in this particular fashion right, so, locally on the gas phase the concentration of water vapour increases locally in the liquid phase the concentration of water vapour goes down right.

So, in the liquid what will happen is that more water will rush towards the interface and more vapour will be drawn away from the interface right. So, this is how evaporation is basically sustained right. So, when you actually have a saucer of water okay.
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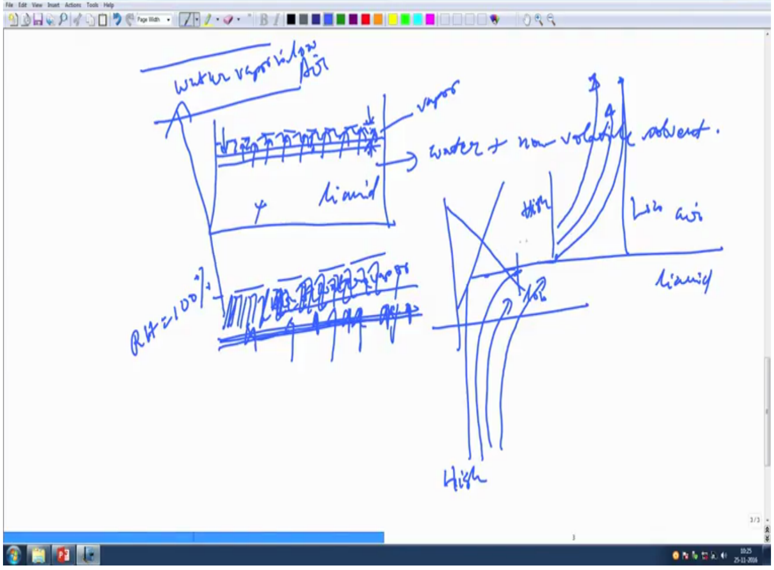

Let us consider this example, so when you actually have a saucer full of water actually. Let us go to the to the journal. Let us look at this and you have a saucer full of water right. So, this is liquid water and say you have mixed it with something right. So, it is basically water plus some non volatile solvent.

Non volatile solvent make it vaporizes very slowly right that is what we mean. This is the interface this is the air okay hanging over there. Now what happens what is the mechanism of evaporation in this case, right. So, that is what we want to answer correct, okay. So, what happens is that locally some liquid water vaporises right from the surface.

It does not happen from here it happens only from the surface layer correct. And it creates an enhanced concentration of vapour on the liquid side, so that is a vapour side, right, okay. So, on the vapour side, so, if I have to plot this on the vapour side, if I just look at this particular distance okay there the concentration of water vapour increases okay, in the vapour side, right.

Whereas on the liquid side the concentration of water vapour actually decreases right, all happening in this small layer okay, so, now if this water vapour is saturated completely I mean this water vapour is present all over right, okay. The evaporation should actually stop correct, okay. This will happen; this is the mechanism; this is because were in this particular location right just above the interface.

If this is the interface just above the interface if you consider that air layer, so, this is air plus water vapour right that is coming and this water vapour source is basically the interface right. Now air you know have got a particular saturation pressure right water vapour has not a particular saturation pressure.

In other words if the relative humidity of this particular section this RH becomes equal to 100 % right. Then what will happen is that so no more water vapour this air can actually accommodate right because it cannot hold anything more. It is already at its full capacity right. Evaporation from this surface will stop okay.

This is what happens when you actually have a very humid environment right, very, very humid like for example if you want to dry your cloth say for example in a very humid environment. Say in during the monsoon okay not because of the monsoon per se but say there is no rain, but the atmosphere is very humid right, so 90 to 95 % humidity okay.

So, that means they the air in this particular region takes a little bit of water and becomes saturated right. So, what is the mechanism for relieving this correct? So, the mechanism of relieving this is if you this is the layer which is very close to the interface right, if you look at a layer which is very away from the interface okay far away from the interface right.

Here what will happen is that here the water vapour concentration is low okay, if it is during the winter season, what it is right now, right. So, in this near the interface the concentration is high. Away from the interface the concentration is low particularly it is a Bangalore's whether it is like 40 to 50 % relative humidity right.

So, water vapour by natural diffusion will go from here to here right that has to happen right. Because it has to flow from a high concentration to a low concentration that is exactly what it does. So, as soon as it does this region now gets relieved okay. It gets relieved right so as soon as this region gets relieved okay more water can come now from the liquid side, got it.

So, this is the general the mechanism of evaporation right. So, here what will happen if we draw it across the interface okay here the concentration of water vapour will be high, away the concentration of water vapour will be low right. So, it is from high to low right, whereas on this side of the interface right on the liquid side so this is the air side right.

This is liquid side right in the liquid side of the interface what will happen it will be just show the opposite trend right. So, this is actually low, this is actually high right, because here the liquid is locally depleted all right, okay. So, this supplies liquid to the interface, this takes away water vapour from the interface, right.

So, long this process continues, your evaporation continues, you got it. This transfers liquid towards the interface for it to evaporate. It takes the vapour phase away from the interface so that this region is we call this as a region right these two regions can be relaxed, got it, okay. So, that is exactly what we have done over here.

So, one other thing is that the gradient of species in go back to the so the gradient of species A in the solid is greater than the gradient in liquids and greater than a gradient in gas this you will always observe. That is because these are governed by the relative mass diffusivity okay so because the mass diffusivity in one case is lower than other and the gas phase mass diffusivity is the highest usually.

So, the gradient will be the lowest rate because it has to match the flux right. For matching the flux there are two things one is basically the diffusion the other is basically what we call concentration gradient right. So, if the diffusion is low then this has to be high okay to match the flux okay.

And usually the gas mixture is approximated by an ideal gas okay. And things like that these are very standard notations okay.

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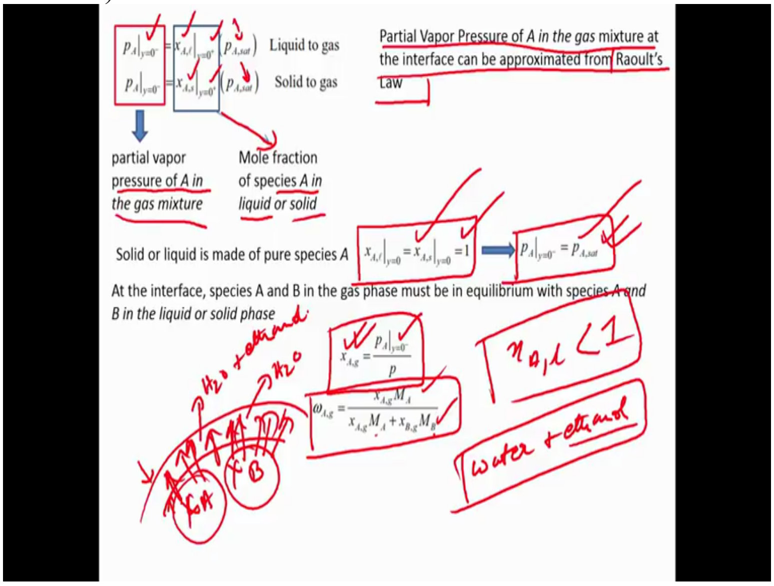

$p_A|_{y=0^-} = x_{A,\ell}|_{y=0^+}(p_{A,sat})$ Liquid to gas

$p_A|_{y=0^-} = x_{A,s}|_{y=0^+}(p_{A,sat})$ Solid to gas

Partial Vapor Pressure of A *in the gas* mixture at the interface can be approximated from Raoult's Law

partial vapor pressure of *A in the gas mixture*

Mole fraction of species *A in liquid or solid*

Solid or liquid is made of pure species *A* $x_{A,\ell}|_{y=0} = x_{A,s}|_{y=0} = 1$ ⇒ $p_A|_{y=0^-} = p_{A,sat}$

At the interface, species A and B in the gas phase must be in equilibrium with species *A and B in the liquid or solid phase*

$x_{A,g} = \frac{p_A|_{y=0^-}}{p}$

$\omega_{A,g} = \frac{x_{A,g}M_A}{x_{A,g}M_A + x_{B,g}M_B}$

Now the other question that you might want to ask that, see we already saw that with curvature okay there was a depression of the vapour pressure right of the saturation pressure that we did in the last class, the last lecture okay. Now here the question that one would like to ask is basically when you have this liquid to gas or solid to gas kind of transition right.

The partial pressure of water vapour in a gas mixture at the interface okay is usually given by something called the Raoult's Law okay. This is called Raoult's Law okay, so this is basically if you look at these two terms over there this PA at y0 - and PA at y0 - these two are basically the partial pressure of A in the gas mixture.

It is the partial pressure of A in the gas mixture just adjacent to the interface that is why you have written that minus right it is just on the other side of the interface, got it, just on the other side of the interface. And this xAl an excess whatever you call it is basically the mole fraction of species A in the liquid or it can be the solid depending on which way you are looking at okay.

And P saturation that you see over here is basically nothing but the saturation pressure at the interface or close to the into at; for which the temperature of the interface is given okay. So, if the interface temperature is ts you calculate whatever is a piece saturation because of that okay. Now if it is pure species like for example as I say pure liquid okay or pure solid.

Now in that particular case this was equals to one this we already established in the last thing right. As soon as we say that this is equal to one the partial pressure of water vapour in the vapour phase okay, is equal to the saturation pressure right. If it is not however which is normally the case with mixtures the vapour pressure is actually depressed that is because xAl is always less than one right.

Because it is a mass fraction the maximum value that it can have is equal to one is always less than one because it is always less than one okay. Because it is always less than one the partial pressure of the vapour phase is actually lowered okay when other species are present that means when you are dealing with say water plus ethanol right mixture got it.

The vapour pressure of water vapour right in the gas mixture at the interface okay will be lower than the saturation pressure, got it, okay. It will be lower it has to be lower that is because you can think about it like a fight right, the space is limited right. So, there is an interface right.

Where you have two species like species A xA and say xB correct both are trying to evaporate and go into that same space right, the space is limited right, okay. So, as it tries to go into the same space obviously if it is alone okay its pressure will be the same as its saturation pressure.

Since it is not alone right depending on what amount of A and what amount of B is present okay. It is pressure that is present in this particular region is consequently lowered its basically common sense right. Pressure is what the number of molecules we can consider in a particular space right.

So, species A, okay is actually evaporating into the same space species B is also evaporating into the same space right. So, they are worth fighting basically for the same space right. Since they are both fighting for the same space right it is obvious that the pressure of species A in that space would be lower than the saturation pressure that species A would have had if it was present alone right.

So, if it is just a pure liquid water droplet that space will be only water vapour right H2O. Now that it has got ethanol okay the; this space will contain water plus ethanol right. It will have the vapour phase of both as a result of that you cannot have the same partial pressure right. So, the mass fraction of species A in the gas phase now can be determined just by that partial pressure that you have determined over here divided by the total pressure.

The total pressure is always the thing okay because of the total pressure is atmospheric right okay. Similarly you can find out other things like mole fraction and things like that basically you bring in the molecular weight because species A and species B are there okay. So, conceptually it should be clear that why evaporation happen this is what we explained okay and how it actually proceed right.

There is a depression of vapour pressure if we are dealing with two species if you are not dealing with two species there is no curvature effect right. We will have the partial pressure of species A to be the same as the saturation pressure okay. So, that part needs to be very clear okay.

So, here we have tried to explain how evaporation happens across the interface okay. So, the next class we are going to look at our particular topic which is basically what we call the droplet okay and the droplet is what we are going to do in the next lecture.