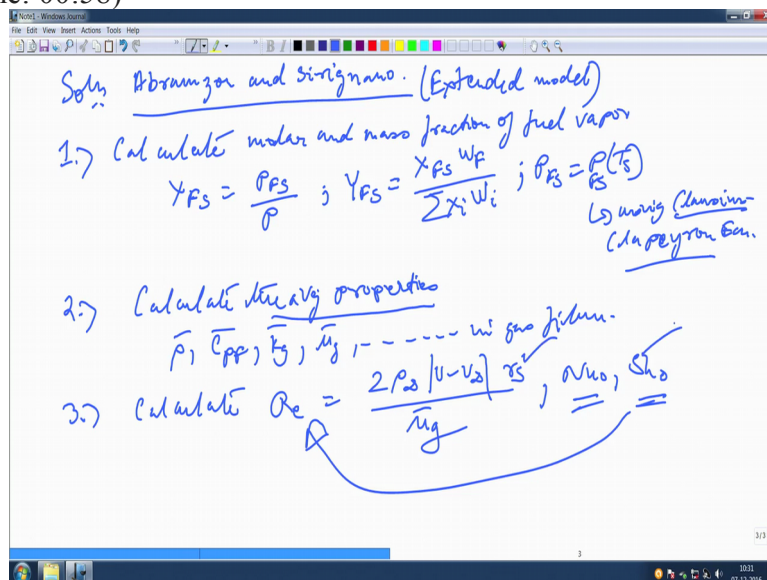


Heat Transfer And Combustion in Multiphase Systems
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Lecture 29
Species transport in droplet

So, welcome to this particular lecture. So, in the previous lecture we showed the insights right that what happens when you use the extended model. What is the difference between the extended model and the effective conductivity model? And how it can predict the temperature and all those other things okay and how what would the isotherms actually look like.

What is the transition between a conduction to a convection and convection to conduction during the life span of a single droplet. It is heavily dependent on the life history of the droplet. It is not just a conduction or a convection dominated problem is actually a mixture. (Refer Slide Time: 00:58)



So, let us look at the solution process that was suggested by Abramson and Sirignano professor Sirignano he is basically the pioneer in the in the work is anything related to droplet evaporation, combustion and things like that both from the modelling as well as the experimental perspective.

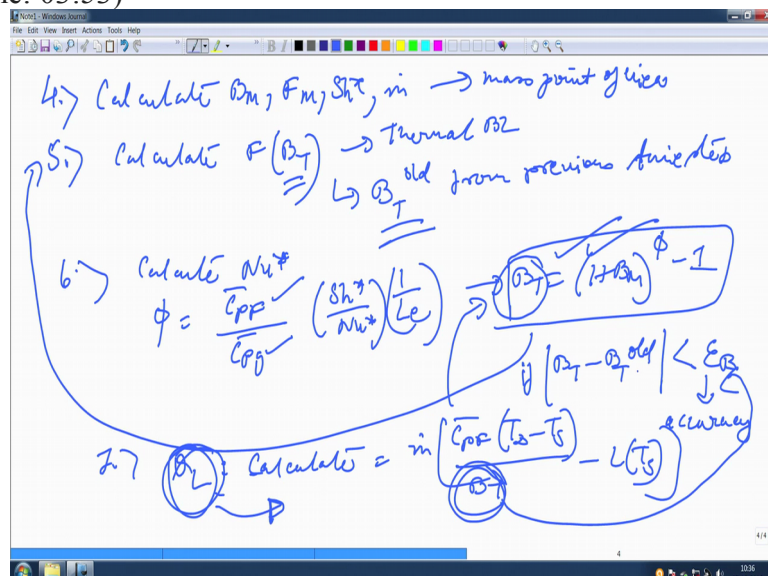
Now that extended model if we look at the extended model how is it solved, how is the extended model actually solved okay. So, we gave you an idea that what is the gas phase what is the liquid phase and what are the outcomes. But let us just give you an idea how this whole thing is solved okay.

So, the first step that people do is calculate and this is solved numerically. So, I am just giving the algorithmic step okay, right. What you do from the gas phase perspective calculate the molar and the mass fraction of fuel vapour okay. So, like X_F is like P_F by P Y_F that is the mole fraction. It is the X_F into the molecular weight divided by summation of $X_i W_i$ right.

So P_F is basically a function of the surface temperature this basically the saturated vapour pressure calculated from the Clausius-Clapeyron equation right, using Clausius-Clapeyron. So, from a numerical point of view these are the steps that one can follow Clapeyron equation. Step two calculate the average property, average properties here means ρ bar, C_p bar, K bar, μ g bar etcetera, etcetera in gas film.

Upto this step it should be fairly easy right this is how you actually normally calculate right, so, using the Clausius-Clapeyron equation to calculate the mass fraction. And the mole fraction okay on the gas side okay. And then you are losing the average properties in the gas film okay. Then the third step is that you basically calculate Re .

This is the gas phase Reynolds number as we know. If you recall that was what $U - U_{\infty}$ rs divided by μ g right. You also calculate Nu naught and Sh naught, you already; we have defined all these quantities earlier these are all related to your Reynolds number that also we showed right. So, you can calculate all these quantities in step 3 right. (Refer Slide Time: 03:53)



So, let us go and look at in step 4 what do you do. In step 4 you calculate B_m, F_m, Sh star and m dot all from the mass point of view okay, all from the mass point of view you are calculating all the quantities like a B_m, F_m, Sh star, m dot and that is the mass flux right.

Then step 5 you calculate F_{BT} that means that correction factor with respect to BT okay that is the thermal boundary layer equivalent.

Using BT_{old} from previous time step you are discretizing it right in terms of time. So, previous time step whatever was the BT value there you are using this to estimate okay whatever is the factor this F factor will be. Sixth step calculate Nu_{star} right Nu_{star} is the is the modified Nusselt number we covered it in the last class.

You also calculate this factor this is the film this is the gas, this Sh_{star} Mu_{star} 1 by the Lewis number okay. And use this to calculate BT , BT is $1 + m \Phi - 1$ right that we already established in the last class also that BT is this okay. Now you return to basically step 5, step 5 if $BT - BT_{old}$ is less than a certain value of this okay.

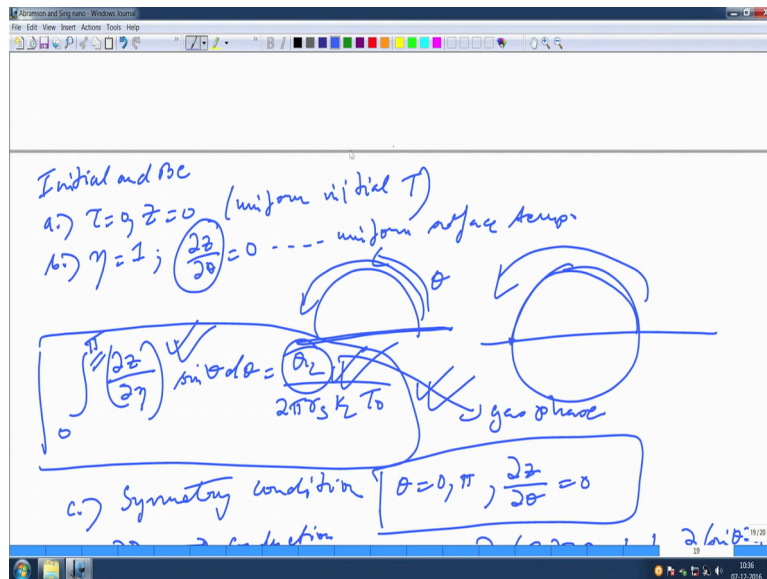
This is basically the accuracy whatever accuracy that you desire okay if you want like a 10 percent accuracy or whatever it is, you actually do it. Then 7th step is you calculate QL , QL which is basically nothing but $m \cdot C_{PF}$ if you recall divided $BT - LTs$ using the value of BT that you got from the previous time step, got it.

Why we are doing this because remember we told you that there is a mass limited or it is heat transfer limited right. In order to have this equilibrium always being obeyed okay you need to iterate over BT okay. So, that it does not over predict if you just use BT as is, right it was over predict okay. So, you are limited by the mass transfer right.

In most of the case would be well limited by the mass transfer. So, you have to use BT accordingly right okay of course when your Lewis number is 1 and other things of course this particular factor does not even come into the picture right this Φ will be almost like 1 okay. So, this is the solution process basically to iterate in the gas phase and find out what will be the value of BT .

What will be the value of QL once you know this value of QL it is very easy because you know where QL happens where QL comes into the picture it comes in through the boundary condition in the liquid phase analysis right. In a liquid phase analysis, if you recall QL was there.

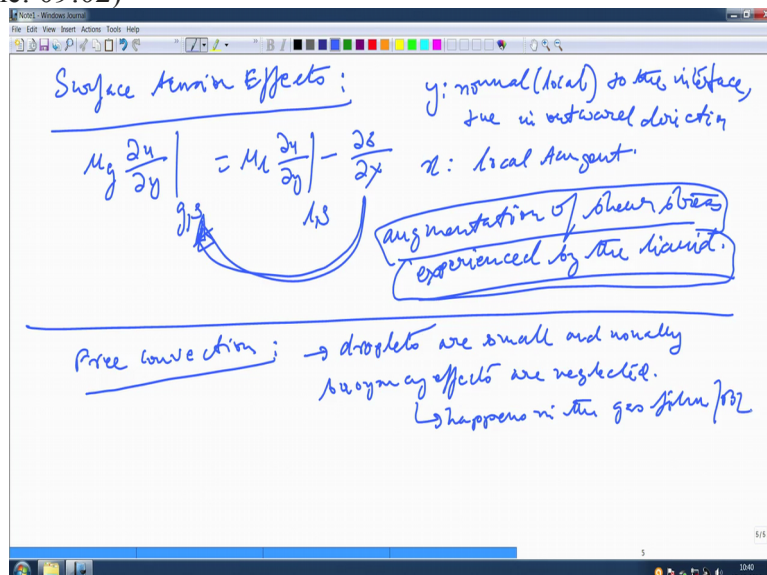
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If you do not let me just pick it up and see here, you see this. So, there is that cool okay, so, QL comes from this gas phase right okay. So, that QL is the QL that you are going to use in here right. So, this QL calculation involves BT but Bt has to be involved in this particular way from the mass and the heat transfer limitation okay.

So it cannot be just worked out like that otherwise you can just calculate BT as is right. But that is not the case because you have to match it with the mass transfer unless you match it with the mass transfer this value will come overly high okay which will be like not the correct thing to do got it, okay. So, this actually tells you that what happens when you actually have to what is the solution process.

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Now let us look at the surface tension effect also remember we said that the surface tension effects are negligible because of the simple reason that there is no variation of temperature the interface. But some people do actually have included the effect of surface tension. So,

what he does is that if you recall your initial classes you will find that this is what happens right.

Gas interface is equal to μ_l the liquid interface side of the interface and then there is a $d\sigma$ by dx right. Here of course y is basically the normal which is a local normal basically local normal to the interface and it is positive okay in outward direction, got it, x on the other hand is basically the local tangent right, okay, local tangent.

So, this is what the equation is actually looks like so the incorporation of surface tension results in an augmentation of the shear stress experienced by the liquid. If this goes to the other side okay if you look at the script goes to the other side then there is an augmentation of shear stress right, shear stress in that liquid experienced by the liquid.

That makes sense now there is an augmentation of shear stress experienced by the liquid. So, what that will do if there is an augmentation of shear stress the surface velocities may actually increase right when you have this kind of an effect into the picture. In addition the surface tension gradient itself can actually generate the flow like Marangoni and this kind of flows okay.

Which we knew that those are the kind of flows that can exist when we first started this discussion, so, all those things can happen, okay but normally when you inject a droplet in a gas flow field okay. There are temperature equilibration around the surface happens pretty fast okay. So, this effect while this can be theoretically incorporated it is not something that is kind of I mean useful so to say okay.

Let us quickly look at the free convection, so what is the free convection normally you know the droplets are sufficiently small to neglect any buoyancy effects right. So, the droplet especially in combustion related applications okay droplets are small right and usually buoyancy effects are neglected correct.

When basically where does the buoyancy effect happens, it happens in the gas film right, this happened in the gas film or the BL the boundary layer right.
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Grashoff Number

$$Gr = \frac{g R^3}{\nu^2}$$

If $R \sim O(100 \mu m)$ at earth gravity
 $Gr \sim O(10^{-1}) \text{ to } O(10)$ --- usually negligible.

$R \sim O(1000 \mu m)$ $\rightarrow Gr \sim O(10^2 - 10^3)$ $\rightarrow$ buoyancy is significant.

1 mm
 mass conservation of liquid
 Piller and Riley $\left[\frac{dR^2}{dt} \sim -R^{\frac{3}{4}} g^{\frac{1}{4}} \right]$ --- numerically done not a representative flow

Now but in some cases it may not be all that negligible. So, in order to define the effect of buoyancy we define a number which is called a Grashoff number, you know what a Grashoff number is, if you do not just open up your natural convection book okay and you can see what a Grashoff number is.

The Grashoff number is basically gR cube writing it big by this right okay. So, it is g is the gravity okay R cube is the whatever, the droplet size that we are dealing with and the kinematic viscosity square. Now if your R is of the order of 100 micron let us say, it is all the order of 100 micron at earth gravity.

The Grashoff number varies from 10 to the power of - 1 to 10 to 10 that is the extent of variation of Grashoff number right. So, this is usually negligible right. So, for 100 micron droplet we can see the Grashoff number is like .1 or 1 to about 10, right. So, 1 to about 10 is usually negligible for most of the case not very significant.

However if R is of the order of say 1000 micrometer okay that this leads to a Grashoff number variation between or the 10 to the power of 2 to 10 to the power of 3. Here buoyancy is significant no doubt about it, here the buoyancy is significant understood okay. So, the Grashoff number of that higher value 10 to 1000 is actually a significant Grashoff number.

So, the buoyancy effect does become very significant in this particular case right. So, it happens in the case of large droplet these are 1 millimeter droplet right. So, 1 millimeter droplet you can have convection effect right. You can have significant natural convection effect okay.

So, from a mass conservation point of view conservation of liquid point of view there were two guys called Potter and Riley they actually found out that from liquid mass conservation they showed that this is the variation when you actually have in the case of this, this is not a separated flow this is a numerically calculated numerically done okay not a separated flow okay.

So, that is a variation that these guys got okay the variation of the R square okay of the droplet basically like the reduction in area of the droplet, R squared is more like area right of the droplet that is the variation that these guys found.

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for mixed mode (NC + FC)
 Fernandez-Pello introduced convection ratio

$$\phi = 4 \left(\frac{Gr}{a Re^2} \right) \left| \frac{T_s - T_\infty}{T_\infty} \right| = \left[\frac{4gR}{a(\delta v)^2} \right] \left| \frac{T_s - T_\infty}{T_\infty} \right|$$

Grashof number

→ Vaporization rate is multiplied by $(1 + \phi^2)^{\frac{1}{8}}$

$$\dot{m} = \sqrt{6} \pi \frac{\lambda_R}{c_p} Re^{\frac{1}{2}} (1 + \phi^2)^{\frac{1}{8}} \frac{B}{(1 + B)^{0.8}}$$

→ $\phi \rightarrow 0 \rightarrow$ pure forced convection.

This is numerical results we are not going through the motions but we are just stating the obvious okay. So, many people then subsequently have undertaken for mixed mode what happens? Mixed mode do you know what mixed mode is? Mixed mode is basically natural convection plus forced convection okay. So, both are actually present okay.

So, for convective heating and vaporization it is a combination of natural convection and mixed convection and natural convection and forced convection. So, Fernandez Pello is a professor in University of California at Berkeley okay. So, he introduced a convection ratio there are many people who have worked we have just picked out one example right.

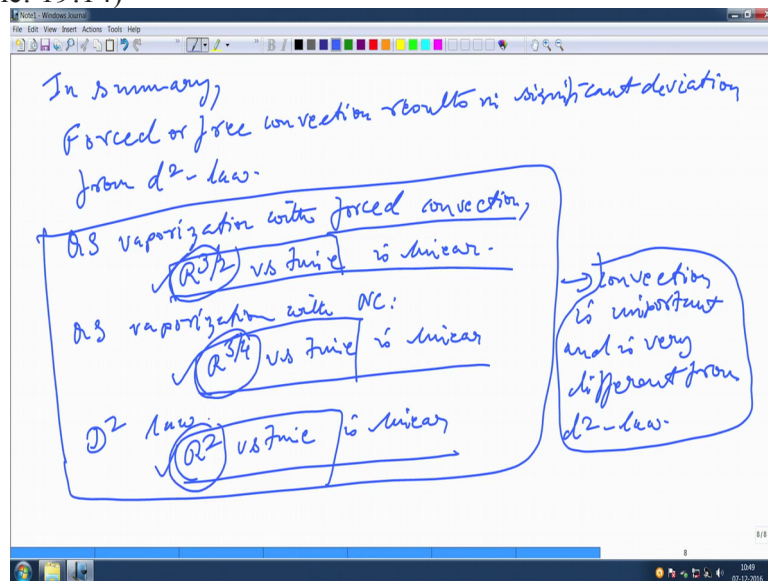
So, he defined a convection ratio called Phi not to be confused to the other Phi's that we did earlier right. That Phi we also compare the sharwood number and the Nusselt number just in a previous lecture should not be confused with that. So, this basically is like a Grashoff number divided Raynolds number square $T_s - T_\infty$ divided by T_∞ is an a, parameter a over here okay.

So, that is the expression, this is equivalent to $4 gR$ divided by $9 \Delta U^2$ because Reynolds number is ΔU , related to ΔU . This is $T_s - T_\infty$ divided by T_∞ bar okay. So, this is nothing but basically the Froude number. So, what he did his convection ratio is basically like a Froude number ratio right.

Just like a Froude numbers right gR by ΔU^2 is by the Froude number okay. So, he found that when we actually use this to calculate the vaporization rate. The vaporization rate is augmented vaporization rate not augmented is multiplied by; so, whatever is the vaporization rate earlier is multiplied by Φ^2 to the power of 1 by 8 okay.

So, the $\dot{m}$ that they calculate 6π by okay so; this is the expression that we found for the vaporization rate okay. So, the vaporization rate is given by $\dot{m}$ into all this kind of quantity right. So, as your Φ goes to 0, right that means this goes to 0, you actually approach pure forced convection, got it, pure force convection.

You go down to pure force convection okay. So, that was what Fernando Pello's, Pello actually found out. Fernandez Pello actually found out.
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So, in summary we have to do a summary the forced and the free convection you can write forced or free convection the results in significant deviation from your d^2 law a significant deviation from the d^2 law right let me that we have seen right. Because for the quasi-steady.

So, quasi steady I am writing as QS, quasi steady vaporization with forced convection what we have is that we have a linear increase decrease of R by 32 versus time. This profile is

linear right that we know this we did earlier right. For similar quasi steady vaporization with natural convection NC results in R to the power of 5 by 4 versus time is linear right.

In the case of d square law we know that R square versus time is linear right, is not that so. So, this is R to the power of 5 by 4 this part to the power of 3 by 2, right. So, there is a significant deviation from that d square or the way of stating all this thing is that convection in whatever form it comes is important right okay.

And it is very different from your standard d square law. If you recall what were the assumptions taking in d square law, you would find out that this d square law is the simplest convection was almost complicated. So, during the course of this few lectures we have gone from the d square law all the way up to the convection.

And we have shown that even if you look at it very global; from a global sense that means we forget about temperature and other things right isotherms other things. You are basically vaporization rate which is related to the reduction of the droplet diameter with time. That varies with R to the power of 3 by 2, R to the power of 5 by 4 and R square depending on which model you are actually using.

So, it is a very different class of problems that is what the emphasis is the most of the things you will find that the d square people just do d square law okay. But there are limitations where is quite a few quite a bit of a deviation. It is not like the even the profiles are actually matching, functional form of the profiles.

If you do not get a d square law just by studying the diameter of your droplets and I mean it makes perfect sense why it should not be that right okay.

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Handwritten notes on a whiteboard showing the derivation of species conservation for a droplet. The notes include the following:

- non-volatile entity: $\frac{\text{salt}}{4} + \frac{\text{water}}{4}$
- Conservation of species:
$$L_e \bar{r}_s^2 \frac{\partial \bar{x}_2}{\partial \tau} + (0.5 \rho_e \bar{v}_r \bar{r}_s - L_e \beta \eta) \frac{\partial \bar{x}_2}{\partial \eta} + 0.5 \rho_e L_e \frac{\bar{v}_r \bar{r}_s}{\eta} \frac{\partial \bar{x}_2}{\partial \sigma} = \frac{1}{\eta^2} \frac{\partial}{\partial \eta} \left(\eta^2 \frac{\partial \bar{x}_2}{\partial \eta} \right) + \frac{1}{\eta^2} \frac{\partial}{\partial \sigma} \left(\sin \theta \frac{\partial \bar{x}_2}{\partial \sigma} \right)$$
- Boundary conditions:
$$\bar{x}_2 = (\bar{x}_2 - \bar{x}_{2,0}) / \bar{x}_{2,0}$$
- Similar energy eqn:
$$\text{as } \tau \rightarrow 0, \bar{x}_2 = 0 \quad \eta \rightarrow 1 \quad \int_0^\pi \frac{\partial \bar{x}_2}{\partial \eta} \sin \theta d\theta = \frac{m}{\pi \bar{r}_s^2 \rho_e \bar{x}_{2,0}}$$

So, now before we finish this discussion okay on the droplet okay, so, now let us imagine that the droplet has now got a non-volatile entity that means they say for example salt plus water, salt plus water salt is our solute water is a solvent right. So, this is water is a non-volatile I mean salt is a non volatile component water should vaporize, salt will not right.

In that particular case if you have to solve this particular problem what you need to do you, need to solve the species equation within the liquid okay. Gas phase already is there right there is this water vapour goes into the air and then we have taken into account the diffusion terms and all those things.

But if you want to do it within the liquid and this is also important for multi-component liquid droplets okay. The same equation will be kind of valid. So, in that particular case if you have say, for example salt water there can be other systems also numerous other systems. We have to; in addition all the equations are valid, we have to in addition write the conservation of species equation.

So, the same equation that we wrote for energy is valid the same equation that we wrote for the outer phase flow field is valid okay except now we have to write the equation for the species inside the droplet. So, here it comes I hope you recall this is once again written in the non-dimensional form everything else is the same.

So, you can just flip your notes and you can see that everything else is absolutely the same. So, this is χ or whatever you call it χ or X just a just a notation thing. So, this is very similar to the energy equation almost identical right to the energy equation by X_z that we have written is $X_z \text{ initial} - X_z$ at any time instant.

This is similar where we had instead of X_z we had temperature in that case right. So, the boundary condition if we have to write the boundary conditions here. So, first the initial conditions and $\tau = 0$ $\chi_z = 0$ right, $\chi_z = 0$ because it is the same as the initial value right when τ approaches 0, $\chi_z = 0$.

Because there is no azimuthal variation of concentration on the surface is one second is the same equivalent definition where we said that the surface temperature is constant right here we say the surface concentration is constant, along the surface. But it is varying within the droplet as well as it is varying with time okay. So, make no mistake about that okay.

So, that part and then the last boundary condition is that n approaches 1 we have $0 \leq \chi_z \leq 1$ by $d\tau \sin \theta = m \cdot \int_0^{2\pi} \int_0^R \rho \frac{1}{D} \chi_z d\chi_z$, okay, so here in the previous case

you had QL if you recall them okay you had QL and your KL and other things, so it is the mass equivalent right.

So, that is these are the free boundary conditions or initial condition and boundary condition that is required to solve this equation right. One initial condition and two boundary conditions are required right because of the nature of the equation right. So, as you have solved the heat transfer you can also solve this mass transfer right.

In addition to this we can solve this mass transfer. So, this is the conservation of species for new species you can write this right n number of species we have to write it for the other components also write the other species component also and you have to know they enter the diffusion of one species into another.

So, it becomes a multi-component diffusion problem which is what is similar that happens in the multi-component fuel droplet. Say for example if you have a kerosene droplet which has got like, got, knows octane, kerosene and dodecane, hexane, in pentane in all this components inside, so in order to study that you have to study the individual volatility of each of the component.

So, this $\dot{m}$ that you see over here will be the $\dot{m}$ for the individual component. So, it only like $\dot{m}_1$, $\dot{m}_2$, $\dot{m}_3$ and $\dot{m}_4$ right and for each $\dot{m}$ you have to find out what is the corresponding BM, BT, etcetera okay. So, that becomes a very onerous task okay not within the scope of this particular course.

But just to give you an insight that when one of the species is our non volatile species you can easily use this equation, the same as your energy equation does not require any other times except that you need to solve this also numerically that is only thing that you need to achieve over here right.

And you know what Nita is all those factors we have already defined earlier, Tau so we defined earlier. So, this actually tells you that how to attack a problem which is of this kind. So, during the course of this in summary what did we do we have started the problem with the pure we defined water droplet evaporation is all about. These are all isolated droplets which by the way and we took baby steps.

We first with the d square law then we slowly cranked up the whole thing and we showed how the gas phase analysis is done. What is Faulkner Skan type of solution there can be right. We also solve the liquid phase we should wrote that what equation is valid for the liquid

phase. For within the liquid phase we argue that the Hill Spherical Vortex perfectly legitimate solution.

And we identified the different regions in the liquid phase like things which one is the inviscid things like that. And based on all the things we have provided our global solution for this particular problem and we have analyzed the data and we have shown what data looks. What we have given correlations involving $m \cdot d$ in terms of Sherwood number and Nusselt number.

So, this also so it has done two things one is that it has provided you with a global perspective that means what is the evaporation rate? How does the diameter vary? At the same time it has provided you the insight that for example how the flow actually how the flow profiles and isotherms are?

What will be the relative variation of the mass flux these things which were kind of not very clear earlier on? These are like what we call inside and these insights have been provided in this particular part of this particular lecture okay. So, next thing that we are going to do is that before we go to atomization of droplet.

We are going to look into, we have looked into like contact free nice spherical droplets. Let us take a little bit of a look okay that what happens when we actually have a sessile droplets into the mix right that means sessile droplets are droplets which are basically on a platform right. So, there is a substrate effect that comes into the picture.

Remember we did that we say that there is a CCR mode and CCA mode and all those things. So, these droplets when they actually evaporate; How do they actually evaporate? Okay and what is the nature of their evaporation? Okay. So, that is what we are going to do in the next lecture okay. So, we end this lecture over here, thank you.