Analysis and Modeling of Welding
Prof. Gandham Phanikumar
Department of Metallurgy and Material Science
Indian Institute of Technology, Madras

Lecture - 14
Solute Transfer Modeling - part 2

Welcome to the part-2 of the Solute Transfer Modeling. This lesson will be on a micro scale modeling of the solute transfer and to visualize that, in the weldment I am just drawing you a schematic here.

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So, this is the melt pool, and this a workpiece. And I am taking a longitudinal section; and as we have seen earlier longitudinal section will have the torch velocity in it; and the torch is moving in this direction. So, you have the melt pool shape like this, slightly trailing effect will be there because of the motion of the torch. And the front side is where the melting is happening; and on the back side is where is solidification is happening.

And it is the micro scale or micro segregation that is happening at the solidification side that we are going to now try to understand; and the domain is not the work piece itself, but a small box that I have shown you here. This box can be replicated at every location on the backside to cover the entire solidified weld, and therefore, it is representative.

And I have oriented the box in the direction of the maximum temperature gradient. The reason being that this solidification is always taking place anti-parallel to the maximum temperature gradient, and therefore, the heater to go this way then the solidification is going in the anti-parallel direction. So, therefore, I have drawn the box along the maximum temperature gradient direction.

So, now you can see that I have drawn a box. So, for now on our domain is basically a small box, which we take it is as one-dimensional; and whatever is happening with in this box can be deemed as applicable within the fusion zone and these box are aligned and stacked to complete the entire fusion weld behind the torch. So, we will take two cases in this lesson; the first case is complete mixing, and that can be discussed as follows.

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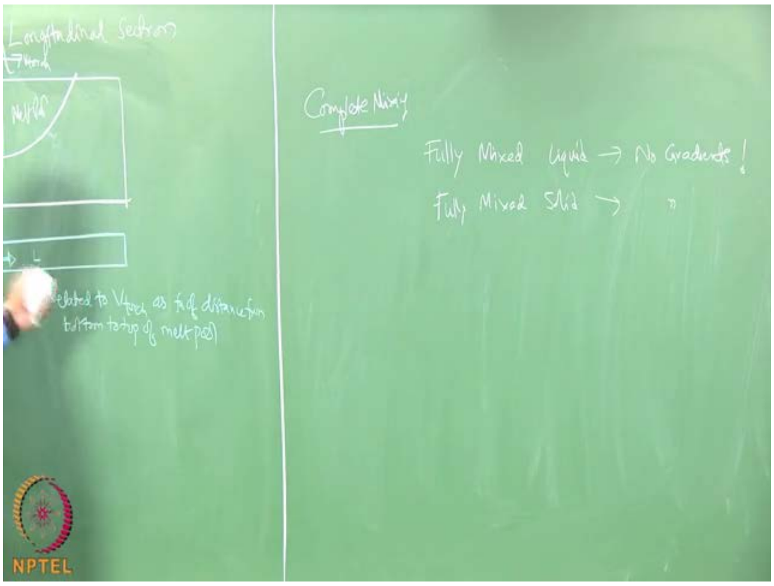

So, before we go there, we can actually just look at the velocity of solidification what we have going to use that is basically related to the angle that the interface between the melt pool and the work piece, namely the fusion zone is going to make with the horizontal and that angle theta can be used to relate V s with V torch. So, at a later point, when we come across what is a velocity here, we should not confuse it with the torch velocity, it is related to torch velocity, but not the same. And it is not also to be confused with a velocity of the liquid pool within the zone here; it is actually the velocity with which solidification is happening.

And you can see that very close to the top, it will approach the torch velocity, but at the bottom it is 0. So, somewhere in between, it will take a trigonometric function like cost theta to change from 0 to 1, and you could actually determine at any location using this angle. So, we will keep that in mind when we need that value.

So, complete mixing assumption is as follows. What we mean by that is within the region fully mixed liquid we have, and also fully mixed solid, this is not generally followed; reason being that normally the solid diffusivity in the solid region is about two or three orders of magnitude smaller than that in the liquid. And therefore, generally it is not possible to have well mixed here in both.

However, we can actually take this assumption and proceed to do an analysis, because it is applicable for small dimensions. So, whenever the length scales are very small this can be taken ass applicable. So, we will look at those assumptions. What we mean by full mixed, so liquid and fully mixed solid is as follows there are no gradients; the solute concentration does not have any gradients, if it is full mixed.

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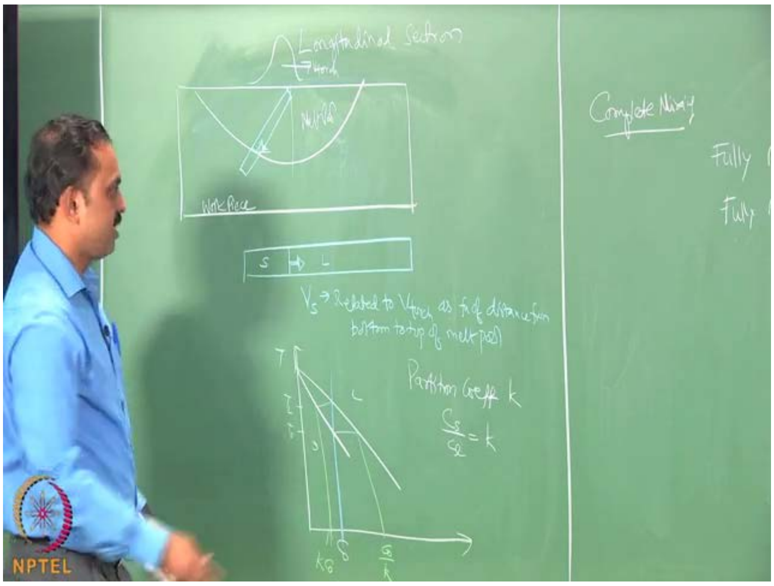

And to go further, we will just also make the phase diagram for this alive for which we are doing this analysis, so that we will refer to the compositions. And we will take a simple you know dilute alloy to make this analysis easier. So, this is the phase diagram. And let us take the alloy which we are going to discuss as this, and starting alloy composition is C naught. And this temperature is the liquidus temperature this is solidest temperature.

And we can say that the alloy C naught is going to start solidifying when the temperature starts going below T L; and it will complete solidification when it reaches T s. And which means that the solid fraction is going to start from 0 at T L, and it will be equal to 1 at T s, so that is the meaning of this. And if this was C naught, then we would introduce what is called as a partition coefficient. Partition coefficient is nothing but the ratio of the solid to the liquid compositions. So, C s by C l is the partition coefficient k. So, as we have seen in the previous lesson partition coefficient, for example, in the case of aluminum copper alloy is about 0.14.

So, you could think of that as value which says that if it is very different from one then this solid and liquid are having very different compositions; and if it is very close to 1, that means, solid and liquid have very close by composition, there is not much the separation solid that is happening. And this also means that you could now find out what would the value of this composition here, what is a first solid that will be coming out, and that can be found out from the same relationship. If the liquid composition is C naught, the first solid composition will be C naught k, k C naught.

And what will be the liquid composition of the last to solidified liquid that is by the time it comes to the end, the solid is having composition of C naught, so the liquid should then be C naught by C l is equal to k, so C l is C naught by k.

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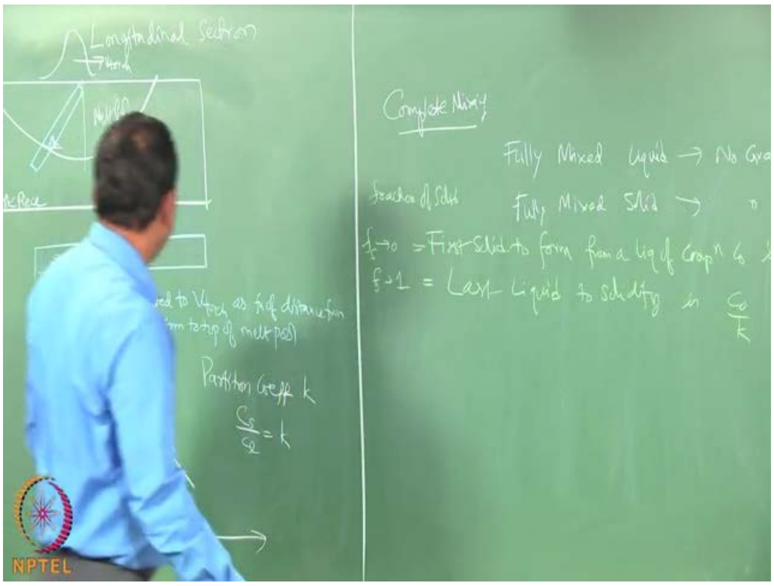

So, which means that I would just summarize first solid to form from a liquid of composition C naught is k C naught; and last liquid to solidify is having a composition C naught by k as we have seen from the phase diagram. So, these values are necessary. And at this point, what would be the f s - the fraction of solid; f s is actually 0, when you are starting to solidify. And here f s is 1, when you are finishing the solidification. So, these are written here, because they will help us in writing the limit. So we will now do the analysis by looking at the solidification of one box subject to the condition that is fully mixed.

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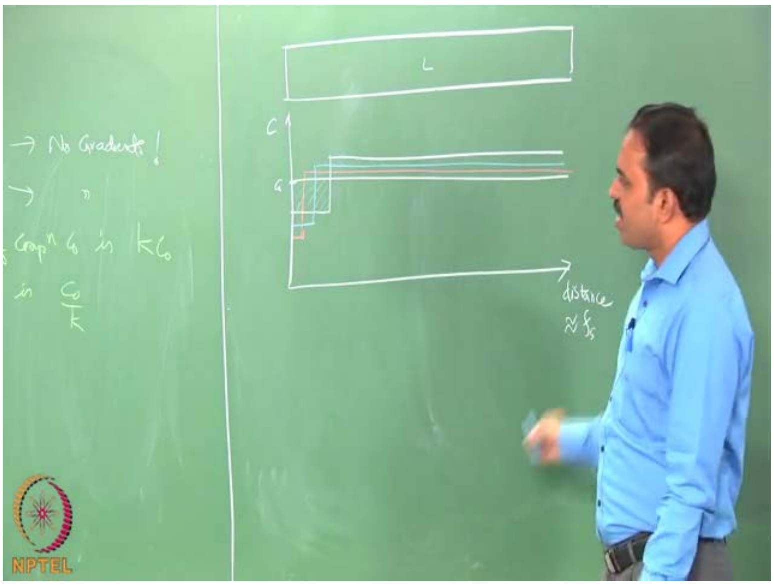

So, let us just draw how the solid profile is going to look like. So, initially this is a box, and here I am putting the composition, and here the distance. And distance can be approximated to the fraction of solid also, because this is entire thing is initially liquid, so therefore, the position of the interface will tell you what is the fraction of the solid. So, let us say this liquid has a composition of C naught then the very first point when you are not at solidified; the composition profile is going to look like that.

This is C naught; it is going to look flats because everywhere the liquids of this same composition. And the moment a small amount, let us say 5 percent of the liquid solidified that 5 percent is going to have a composition of k C naught, and k being 0.14 for aluminum copper, it means it is going to be a small value here and this much of solute has to them mix in the liquid. So, the solute when it is mixed will have the composition of the liquid going up.

So, this will the profile of composition after some amount of let us say 5 percent of solidification has happened, the profile is not flat fully, it is two steps; one step here and then another here showing a slight increase, because this much of solute has to be dumped across the entire width of the box.

And if you again solidify another 5 percent then what happens is that it would dump some more. And solidify 5 percent then and it can keep going like that. And what happens is that when we are assuming that this region is fully mixed, it means that within the solid this kind of steps are not allowed, there are fully mixed. So, therefore, we would just draw them all the way to end. So, every time the composition in solid is adjusting and this much of solute in this box, let us say this box is distributed on the other end, so that it can be balanced.

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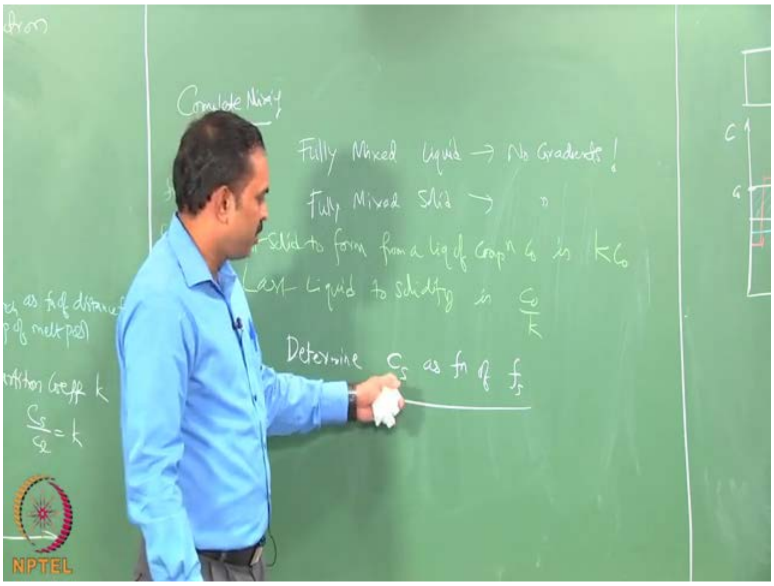

So, now to understand how the composition is going to vary when the solidification is going, we pose the problem as follows. What is the problem the problem is basically determine C s composition of the solid as a function of f s. And you can actually pose it as determine the composition of the liquid as a function of the liquid fraction whichever way because both are related. And we can then use this plot to determine that.

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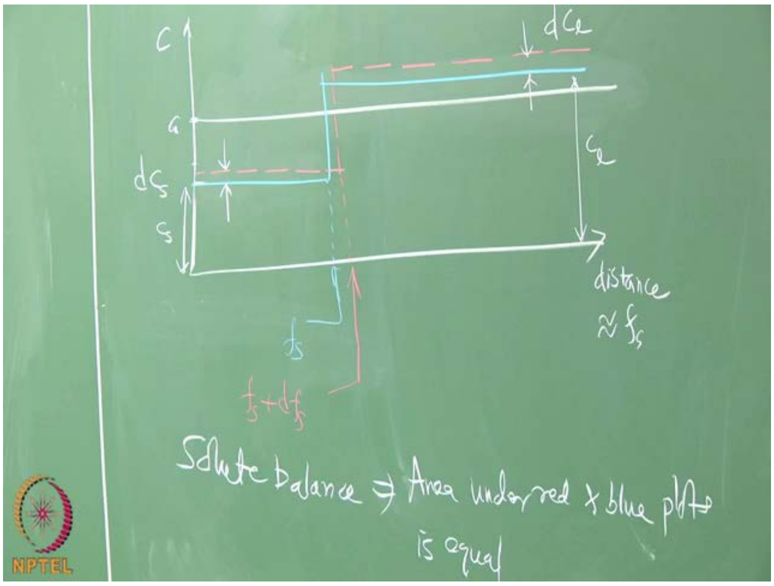

So, what we do is that to determine, we go from comparing situation at f s to f s plus d f s which means that let us say from 20 to 21 percent that kind of a small variation in the solid, and let us look at what will happens. So, I would just take two sets of lines. And I would exaggerate the d f s, so that is visible in the board and then show you how the profile should look like. So, let me just draw that for you; C naught is still flat and composition is here, and after some amount of solidification little bit, so that will be the one, which means that this value is f f, and this value f s plus d f s.

And when the solidification has gone from f s to d f s that is 20 to 21 percent let us say how much the increase of the solute concentration has happened. So, which we means that gone from here to here, and this increase in the concentration of the solid can be thought of as d C s, so that this composition is C s. And this increase in the solid liquid composition can be seen as d C l, so that rest of it is C l. And these expressions will still be valid, the definition of partition coefficient and all those things are valid.

Now we then perform solute balance which is basically to conserve the amount of solute that is there. And solute balance should then be written in such way that the area under the blue curve is equal to the area under the red curve. So, that is what is solute balance implies the area under the red and the blue plots is same that is when the solute conservation has taken place. So, let us then write expressions that would make that conservation possible and then we would write that expression here, so that we can make the derivation. Let me erase this part and then show you how that expression look like. So, the area under the blue curve can be written as two rectangles, this rectangle would then be C s into f s.

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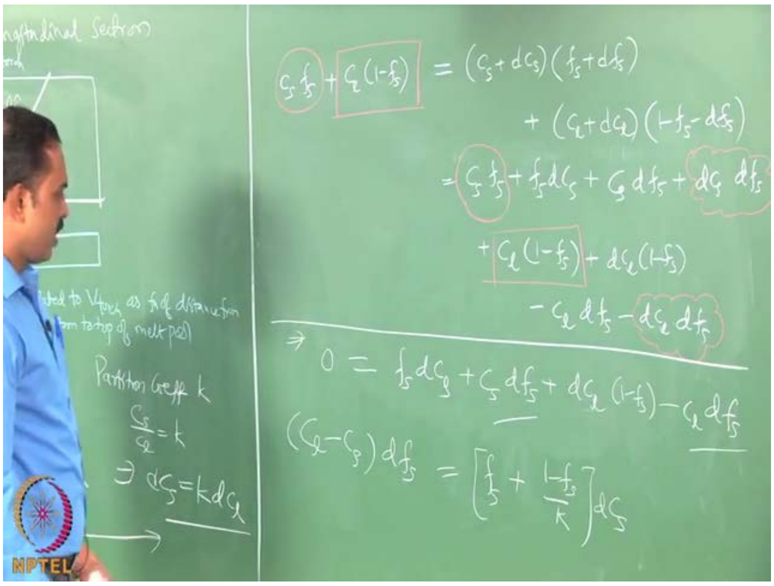

$$C_s f_s + \boxed{C_l(1-f_s)} = (C_s + dC_s)(f_s + df_s) + (C_l + dC_l)(1 - f_s - df_s)$$

$$= C_s f_s + f_s dC_s + C_s df_s + dC_s\, df_s + \boxed{C_l(1-f_s)} + dC_l(1-f_s) - C_l df_s - dC_l\, df_s$$

$$\Rightarrow 0 = f_s dC_s + C_s df_s + dC_l(1-f_s) - C_l df_s$$

$$(C_l - C_s)\, df_s = \left[f_s + \frac{1-f_s}{k}\right] dC_s$$

So, it would be C s f s plus, the rest of it is basically C l into 1 minus f s, this is the area under the blue. And the area under the red is going to be having the height slightly more and that would be written as C s plus d C s that is a slightly increased composition and that has solidified up to f plus d f s plus the area under the red curve here would be having height slightly increased, so C l plus d C l into the length has actually shrunk a little bit and that can be written as 1 minus f s minus d f. So, these two areas being same implies that when you multiple with the uniform cross sectional area then you are actually solute balance is being applied.

We would then expand only your right hand side, because we can see some cancellation that is possible. So, we would then take only these terms and see. So, C s into f s plus f s into d C s plus C s into d f s plus d C s in to d f s. And then this again we will write it as plus C l into I intentionally keep 1 minus f s together, so that I can cancel it later on, and then plus d C l into 1 minus f s minus C l into d f s minus d C l into d f s.

Now in this expression, we can note that we can start canceling of terms and then I will highlight them. So, this is same as here, so that can be canceled; and this is same as this that can cancel; and then you can also see some more things can be neglected. So, usually these double differences are extremely small numbers, because both are suppose to be small. So, I would then neglect those second order effects. So, those can also be dropped, which means that you can now write this balance with only the remaining four terms which can be collated. So, I will just bring them across and see how they look like.

So, this implies, so zero is equal to so f s d C s C s d f s plus d C l into 1 minus f s minus C l into d f s. Now what we need to do is basically identify the terms that has same differential and being them together. So, they have the d f s as common. So, we just bring it to the right hand side. So, we write it as C l minus C s into d f s is equal to on the left hand side you have the T d C s and d C l that are together. So, we could use the definition of partition coefficient to write saying that implies d C s is equal to k into d C l, we can use it, so that we can change it. So, it can be written as f s plus d C l is d C s by k. So, this is the expression we have now arrived. So, now, you could at then make this little bit more simple by using the same expression.

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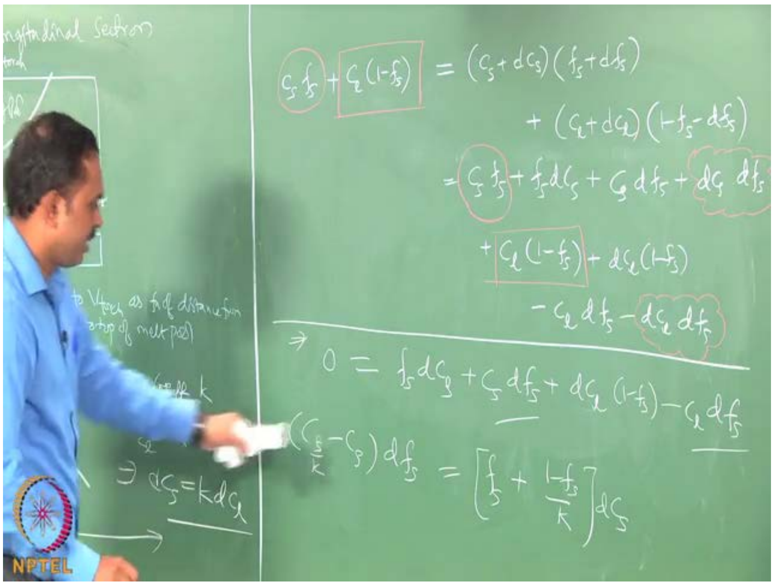

So, you can already see that C s by C l is k which means that this can be simplified.

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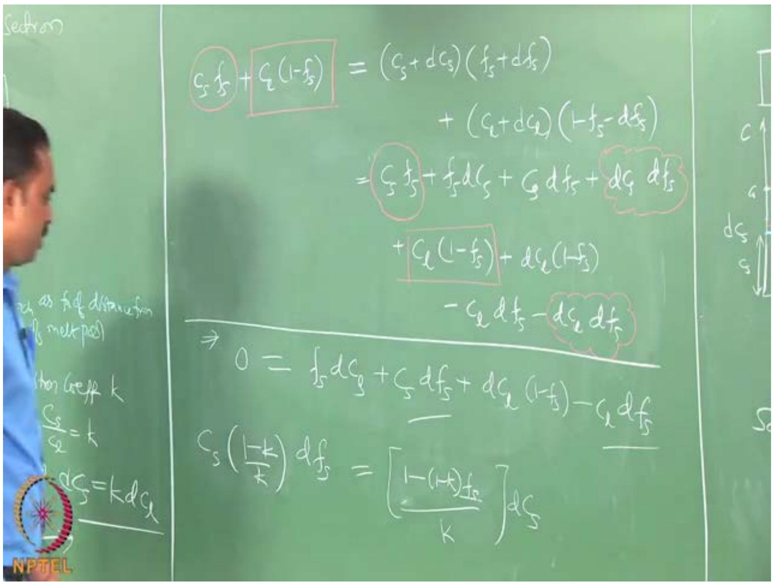

So, this can be written as C s by k, which means that I can take the C s out. So, I can write like that and here also I can make a simplification and that I would do by multiplying.

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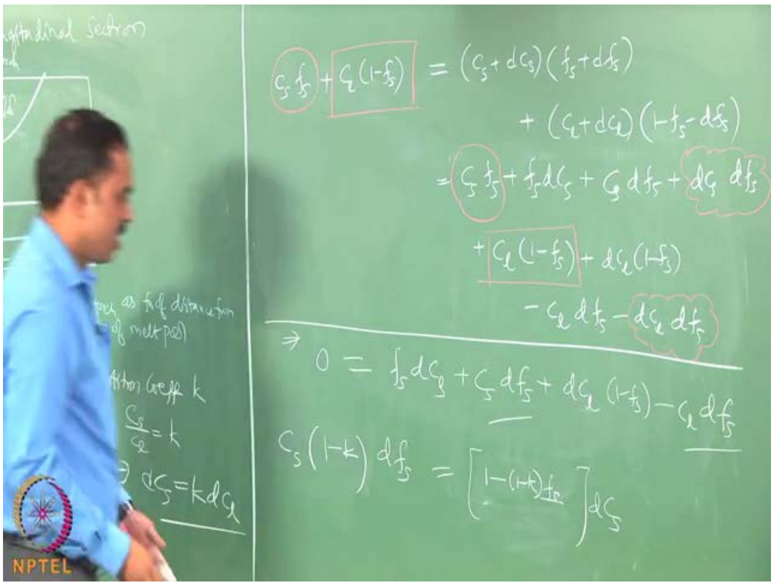

So, I would take the k fully down, and I put a k there. And then I can take the f s common, so that would be 1 minus 1 minus k l. So, this is how it is written. And now you can see that both sides have a denominator k, so I can ignore that. And you can see that when you want to integrate you normally should have the same variable along with the differential, and so which means this square bracket should be brought down here, this can be taken to the other side there. So, we will do that manipulation now, so that we can integrate.

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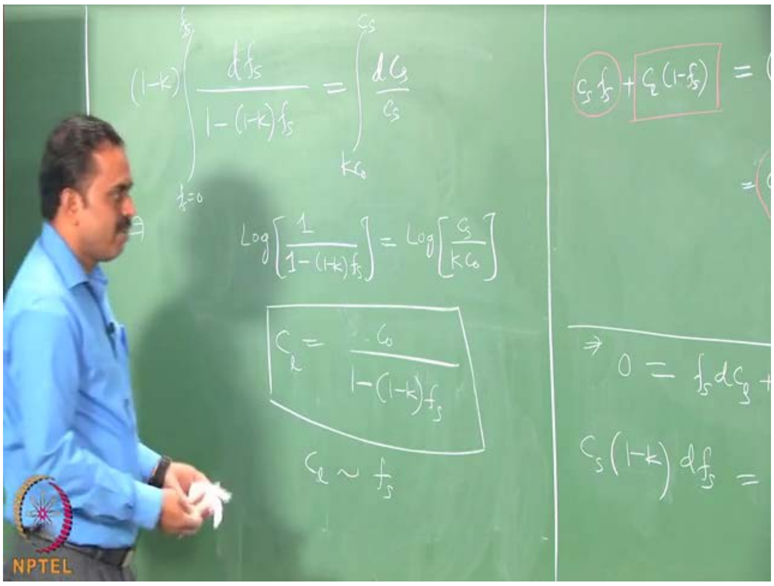

So, let us just manipulate this. So, d f s by 1 minus 1 minus k f s, and 1 minus I have just still keep that here is equal to d C s by C s. So, now, for you could see that you have the same variables nicely grouped. So, we could integrate these. And you could start from f s is equal to 0 to f s is equal to f s; and at f is equal to 0, the solid composition is given by k C naught; and at f s is equal f s, the solid composition is given by the C s which means that we can now integrate and substitute these limits, and see how the expression is going to look like. And therefore, we can see that it comes as logarithm, and let us just substitute that it implies 1 minus k logarithm and the minus sign here, which means that I can swap the integrals signs, and therefore, 0 should be the first limit and therefore, it should be coming as 1 0 here.

And then f s is the second limit 1 minus 1 minus k f s is equal to log. The first limit is still here it is log C s first limit is C s, second limit is k C naught. And you can see that the 1 minus k has been here it should be absorbed. So, you remove that fellow here, because it supposes to be one minus k as the multiplicative factor here. So, which means that if you exponentiation both, you start seeing how the expression look like and we would do that now. Which means that you would see that C s is equal to k C naught divided by 1 minus 1 minus k f s and C s by k is nothing but C l which means I can write it as C l is equal to C naught by this.

So, this is an expression which tells you how C l is related by f s. You can also call it as C s related by f s, because you can write it as k C naught by 1 minus 1 minus k f s etcetera. And this relationship, the way we have written is looking like a function as you vary the liquid fraction how the concentration of the liquid is changing etcetera. Now in this form, it may not be recognizable immediately what it is, but we would just simply manipulate a little bit and show you what it means.

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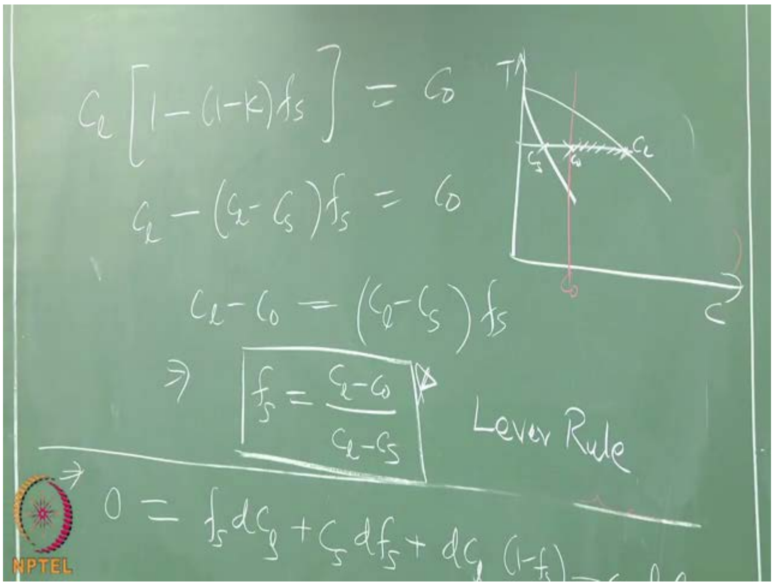

So, what does balance of solute mean is being demonstrated. So, what we do is that we will just take this expression and manipulate. So, you would have the expression C l into 1 minus 1 minus k f s equal to C naught. So, I will write it as C l minus 1 minus k C l minus k C l into f s is equal to C naught; k C l is again C s. So, you write it as C s. So, then you can take this C naught there. So, you write a C l minus C naught is equal to C l minus C s into f s. It implies that f s is equal to C l minus C naught divided by C l minus C s. Now is this then clear what it is; for you to recognize this, I would just quickly draw the phase diagram and show you what we meant.

At a given fraction, if this was C l, and this was C s, and this is C naught, then what we have written is C l minus C naught that is this distance divided by the total distance Lever rule. So, lever rule is nothing but balance of solute, under the assumption that you have got complete mixing in the liquid and in the solid region. So, there is absolutely no special phenomenon behind this equation Lever rule, it is actually giving you the function of the liquid composition as a function of the solid fraction or liquid fraction. And under the situation that is fully mixed in both solid and liquid, you retrieve the Lever rule. So, this is one thing that we can bring from the relationships that we have drawn.

And when is it applicable, whenever the complete miscibility is there in the liquid, which is generally not possible in a fast process such as welding that is reason why Lever rule is not applicable most of the time to understand what would be the composition variations that are happening at micro scale. And we now see that it is originated because of assumptions that we started off. So, we can now modify this equation to relax at least one of those assumptions; and the first assumption that we would like to relax is the composition equilibration within the solid, because solid normally has very poor diffusivity.

So, you can reduce the amount of mixing in the solid by simply setting it to zero, and then look at it we would just take a short break. And we will come back to this derivation and see how this equation would change if we make that relaxation. So, let us get started back from the previous part on the second part of the solute transfer modeling which is applicable for the micro scale redistribution of solute because of the solidification of fusion weld meant. So, here we have seen that in the previous part, we have derived essentially a Lever rule by assuming complete mixing in the solid and liquid region.

And we have seen that it is applicable only when we have got very close while conditions for equilibrium to be set; and for a fast process such as welding, it may not be applicable. And we will relax one of the conditions to make it bit closer to the reality by saying that we will use complete mixing in the liquid, but no mixing at all in the solid which means that you would have a situation of variation in the composition as follows.

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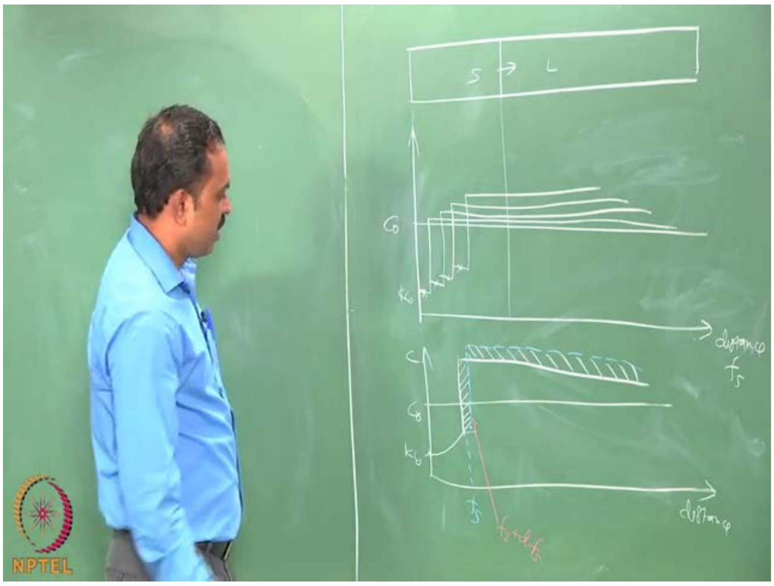

So, a schematically the way we have draw earlier, we would do the same thing here. So, this is nothing but the distance r d f s. And what would happen is that initially we are saying the composition is taken as some C naught; and because of a small amount of solid that would form initial composition can be k C naught. And the plot would look like that because this much of solute has to be then distributed in the liquid. And the next delta of solidification would intend that it should be like that; and then further on, it should go like that.

Unlike, in the previous section, where we said that the entire solid is also having fully mixing, so that the composition is made as flat; in this case, we will not do that; we will say that there is no diffusion in the solid which means that the profile of composition variation in the solid will just stay frozen as we have given. So, a step-by-step profile like this, if you take the middle points would show that it is actually an increasing plot.

So, we can then redraw this profile by making it smooth as follows. So, if this was the case C naught C as a function of distance, then the profile would look like this, this is k C naught. And what we are trying to then balance is when the liquid fraction is going from f s to f s plus d f s. And let us then draw them like this. This is f s plus d f s and the composition has gone from C s to C s plus d C s, C l to C l plus d C l by a small change in the solid fraction that has solidified.

And the solid composition is not getting equilibrated it is some arbitrary curve that is depended upon the process conditions. So, we will not bother about the nature of that curve to do the solute balance. The solute balance requires that the area under the white line and the blue line should be equal. And we see that some of them are constant common to both. So, this area is common to both, and this area is common to both. So, which means that you can actually look at only two regions, and then make them equal; and I am shading them here.

Because of this solidification happening by making the solidification go from f s to f s plus d d f s, it has changed only this much; that means, if this hatched region is equal to that hatched region then the solid balance is maintained. And while maintaining that we will also see a lesson from the previous class that the product of d f s and d C s are negligible. So, this corner which is basically like a triangle is can be now neglected, because f s C and d f s, and d C s are very small. So, we would just pretend that these two are essentially rectangles, and look at their balance.

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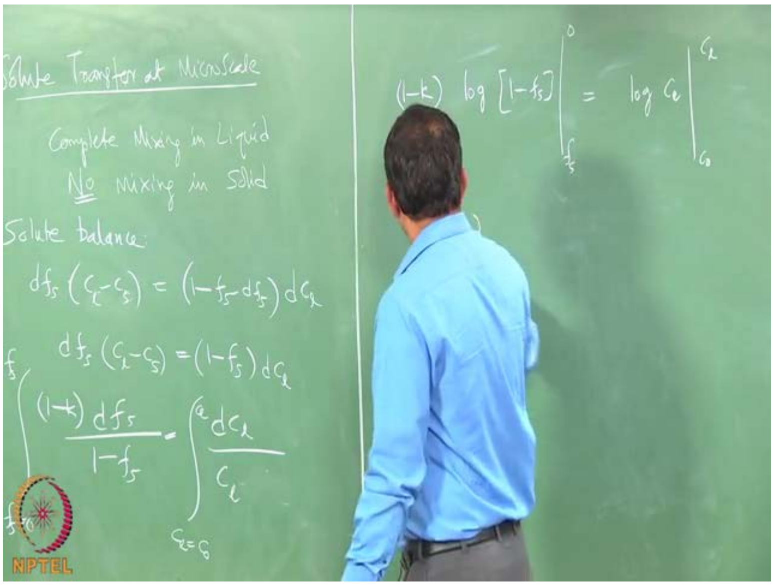

So, solute balance would require this So, the vertical rectangle this part is basically the width is d f s; and the height is nothing but the liquid composition minus solid composition, which is C s minus C l, that is the area. And the horizontal rectangle here would then have the width which is nothing but 1 minus f s minus d f s into the height; height is nothing but d C l. Again we see that d f s and d C l are getting multiplied here, we can ignore that. So, we could write this simply like this; d f s into this is the height difference is C l minus C s, because you are approximating the double differential products as negligible.

And we can then bring the quantities on either side to see how they express themselves. So, you could write it as d f s by 1 minus f s is equal d C l by C l minus C s. And we can also see that C l minus C s can be made as a function of C l itself. So, you could take C s as k C l. And if you take the C l as common, so you could write it as C l into 1 minus k and that 1 minus k can be absorbed here. So, you have that equation.

So, this has to be then integrated to see how the variation of C l with f s is going to be. So, you would then put that integrals and initial condition, you can say at f s is equal to 0, what would be the C l is equal to C naught. And when f s is equal to f s, C l is equal to C l. So, you can then immediately see that you can integrate, and it would look like this 1 minus k into log 1 minus f s. And the integral signs have to be swapped, those 0 will be here and f s will be down because of the minus sign here and is equal to the next sign will be log and C l the top will be C l bottom will be C naught.

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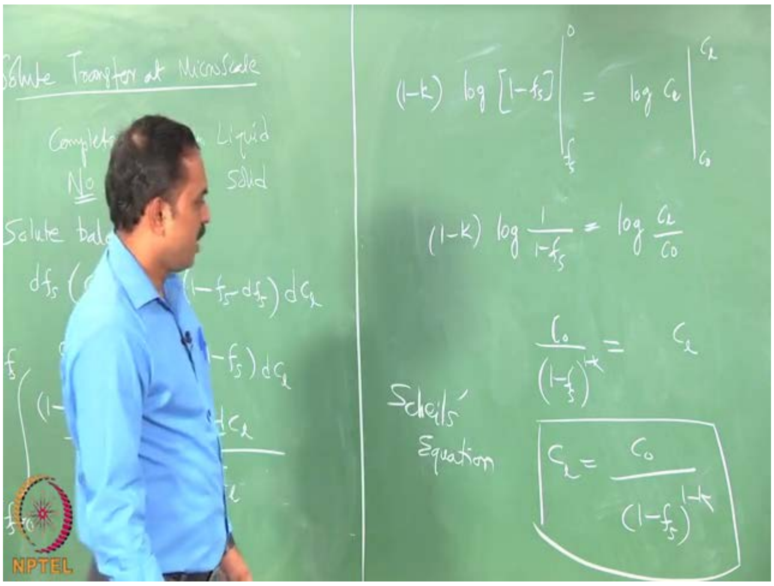

So, which means that 1 minus k into log 1 by 1 minus f s is equal to log C l by C naught. So which means that you can take this as an exponent here, so log 1 by 1 minus f s raise to the power of 1 minus k is equal to C l minus C naught then you can exponentiate both sides to remove the log. And then you can bring the C naught here, so that you can see that the expression is given as C l is equal to C naught by 1 minus f s raise power of 1 minus k. So, this is expression, I will just write it again C l is equal to C naught by 1 minus f s raise power of 1 minus k.

This expression goes by the name Scheils’ equation. So, it is different from Lever rule where you do not have the exponentiation; Scheils’ equation you have an exponentiation. And you can see that for values that are of partition coefficient like 1.14 then basically this is a positive power and 1 minus f s would mean that the liquid composition is rapidly rising above C naught as the solidification is coming to end.

And how we can apply the Scheils; equation to derive the eutectic fraction when you have, for example, towards the end of the solidification even though you are expecting detective to form for the alloy composition that you have chosen that can be used. And the way you do it to find out is just substitute for C l, the eutectic composition and find out what would the f s.

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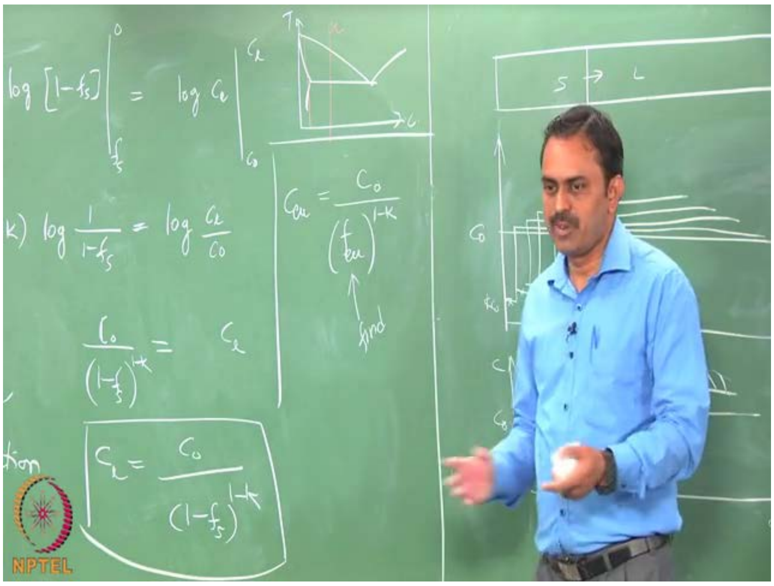

So, we could do that very simply here, I would just illustrate here. If C u eutectic was known then you can C naught and what was supposed to found out eutectic fraction which is the liquid fraction this is f s is solid. So, you can say f eutectic is nothing but f l base the power of 1 minus k. So, you have the initial composition, you have the eutectic composition, you have the partition coefficient, so find this and then you get what would be the eutectic fraction remaining during welding, in case the welding is happening under the regime, where the Scheils’ equation is applicable, which is actually quite reasonable to expect.

And you would see that you would get a reasonable value for eutectic fraction, even though the phase diagram does not give you the eutectic at all and it is also know in the experiments that alloy compositions which are slightly you know ahead the limit - the solidification limit, I would just draw them here.

So, for compositions like this you do not expect any eutectic to form, but then if it where any welding situations, you would have eutectic to form. And normally equilibrium predicts that only this kind of a composition will have eutectic, and these should not have, but then you would see that eutectic can be absorbed immersed on such alloys and how much it will absorbed can be given by the Schiels' equation. We can actually see the behavior of Schiels' equation through couple of exercises in the tutorial that I would be putting up in the course website.

And with that, I will close the second part of the micro scale solute transfer at this juncture. And in the next lesson, we will see how we can actually relax one more condition that we have set here namely the fully mixed region in the liquid. We can relax even that and then see how the solidify aggregation can help us in understanding how the solute distribution will be happening at micro scale and also how it will affect the micro structure.

With that, we will close this lesson.

Thank you.