Analysis and Modeling of Welding
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Lecture - 15
Solute Segregation Profile - part 1

Let us start the second set of session Solute Transfer in weld pool. So, we are going to look at the solute segregation profile and we will do it in two parts.

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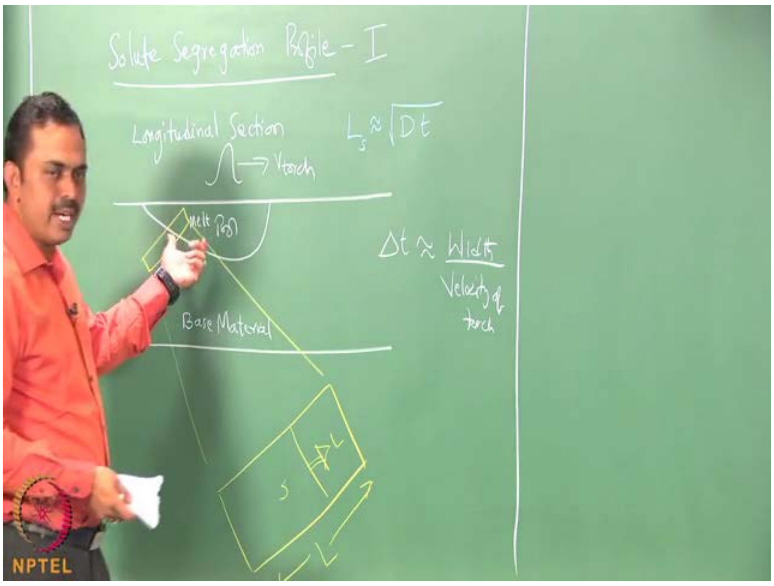

The first part, we are going to look at the overall nature by which we are going to proceed further having considered already the lever rule and the Scheil's equations. So, here is the situation that we looked at for the domain. So, here is the melt pool the heat source is moving, and we are looking at the longitudinal section; and in the weld pool, you have usually a trialing effect and that means, that ahead of the center of weld pool you have got the melting process taking place and behind it is a solidification process taking place.

And I have drawn a rectangular domain which is in the direction of maximum temperature gradient, so that it captures the direction of solidification of the weld pool.

And I have enlarged it to show you that in this particular rectangular shaped small domain we have almost a directional solidification that is taking place. So, therefore, it implies that if we can understand the microstructure evolution of weld pool within this domain, then we can apply it to the rest of the weldment, because we can imagine the solidified weld behind has comprising of this tacking of these kind of rectangular domain one after the other.

The domain that we are looking at is much smaller than the actual weldment, and this must be kept in mind. So, before we put the lever rule, and the Scheil's equation into a prospective, let us appreciate one thing that the length scales are very small for solute diffusion to take place. The diffusivity as we have written here for the solute element, let us say for example, the diffusivity of copper in the case of aluminum copper welds, for example, will be very small and when we take the time available for the process of the solidification then we get what is called as length scale of diffusion. So, this is a length a scaling analysis that we have shown.

And here what do we want to use for the time we can use the time that is meant for the solidification process which could be estimated for example, the delta t can be estimated as the width of the pool divided by the velocity of the torch, which means that that is the amount of time that is available for the melt pool to solidify completely beyond that the torch has gone further away and that if that is a time available. And then if that you substitute here then you get the length scales over which a diffusivity is going to play a role and the segregation are going to be event out.

So, this length scale will tell us whether further features that we are looking at are it sufficient for the mixing to happen or not. In other words, let us say for the feature we are looking at let us say the side arms spacing or the primary generate arms spacing etcetera then if that length scale if we are looking at is smaller than this number it means that the mixing is possible in the complete sense. If it is larger; that means, mixing is not possible completely. So, in that, we can actually see what comprises about good mixing or poor mixing.

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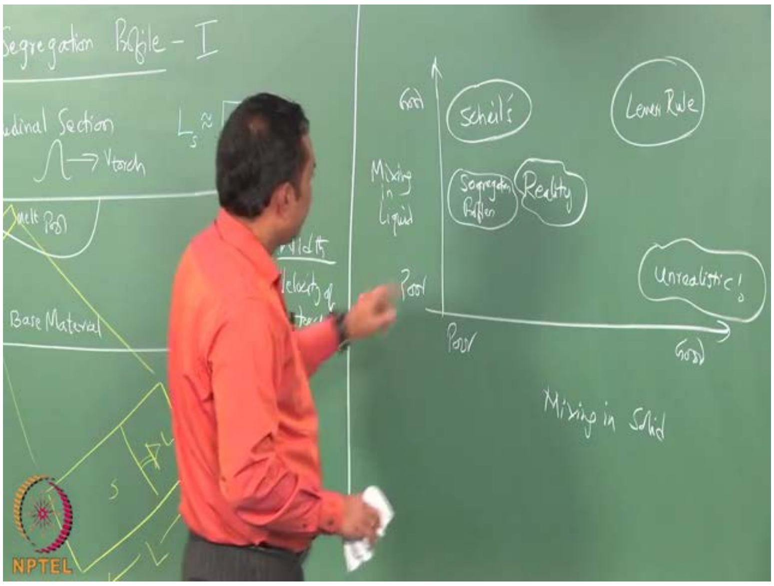

And we can just put that into a map. We can say it is here on the x-axis, we can say mixing in solid; and on the y-axis, let us say we put in mixing in the liquid. And what we mean by this corner is let us say poor mixing, good mixing, and here also poor mixing, and good mixing.

So, what we meant by lever rule is we assumed that the mixing in the solid is perfect complete and mixing in the liquid is also complete, which means that in this domain it is here that we are getting the lever rule; it is good in both. And then we made one relaxation to this particular set of assumptions when the derived the Scheil's equation we said that the solid has no change in the composition during the solidification of the weldment and liquid still has very good mixing, so which means that as far as Scheil's equation is concern, we are here. And we would also see that there is some domain that is not possible.

It is very difficult to imagine a situation where in the solid very good mixing is there, but in the liquid it is not there because that is very unlikely the reason being that in the liquid the atoms are having transnational freedom, they are jumping around; whereas in solid they are sticking around with their own lattice position. So, very difficult imagine a situation. So, we can say this is unrealistic. And where would the reality be, the reality would be such that the mixing in a solid is slightly on the poorer side, and the mixing in the liquid is good, but not completely available. So, such if we can say reality is may be here. And what we would like to take up in this lesson is here, where the mixing in the liquid is not complete, but it is also not totally neglected, it is not 0, so it is available and in the solid you just. So, completely ignore it.

So, we are trying to take a some situations which is quite close to the reality, and this is the place where segregation profiles are going to be there. As you can see that it is in the realistic situations that you have basically some amount of back diffusion in the solid behind the dendrite, and you also have for example, some amount of mixing which is not complete. And you can say what is intermediate it means that diffusivity is such that it is not fully mixed and it is determined by the diffusion coefficient.

So, we can say that we can take a situation now which is quite close to the reality. And this is equilibrium situation extremely slow solidification of welds may be submerged arc weld, for example, you may take this kind of a situation. And for all practical proposes most of the welds like in a plasma arc welding and upwards, you may see that it is quite difficult for the liquid to have a enough time to mix. So, you may actually take Scheil's equation regime and that may be quite realistic and otherwise you would say that this is the profile that we can use. So, what do we mean by the segregation profile is as follows.

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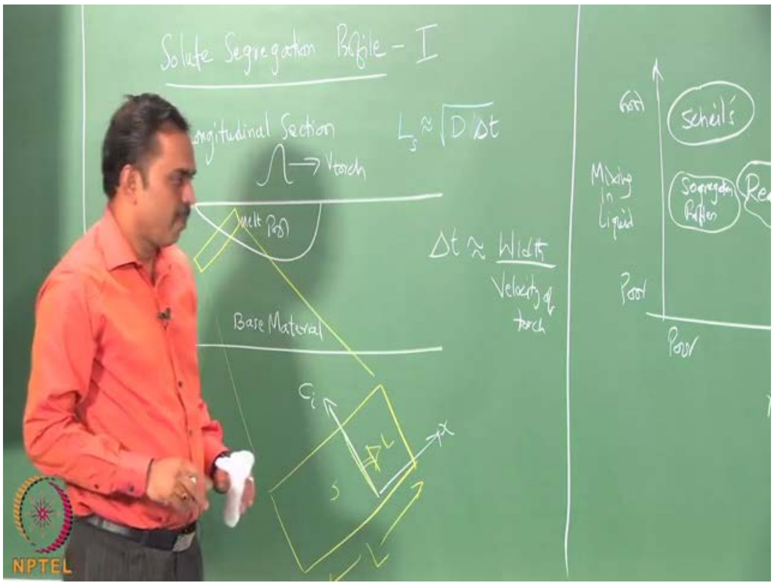

We are interested in as a function of distance along the domain that we have drawn what would be the composition of the solute that we are interested in. So, if this was the distance, we want to plot the composition of the solute. And that would tell us various things including what kind of microstructure we will get in the weldment, and also to tell whether there would be a banding, and in which case in those bands whether there will be possibility of inter metallic compounds to form etcetera. So, there is large number of things that you derive from a solute segregation profile that you can draw.

And the way we would propose the solution is as follows in the case of the derivation for lever rule and Scheil's equations, we have taken fixed length of the box, and we have taken the solute balance. But in the case of the solute segregation profiles, we are already saying that the mixing in the liquid is not complete, it is inadequate. So, we are going to assumes that the domain is roughly about three to four times the length scale of the diffusion, which means that it is the approximated as a semi infinite domain. So, I will just write down the conditions under which we are going to do the derivation.

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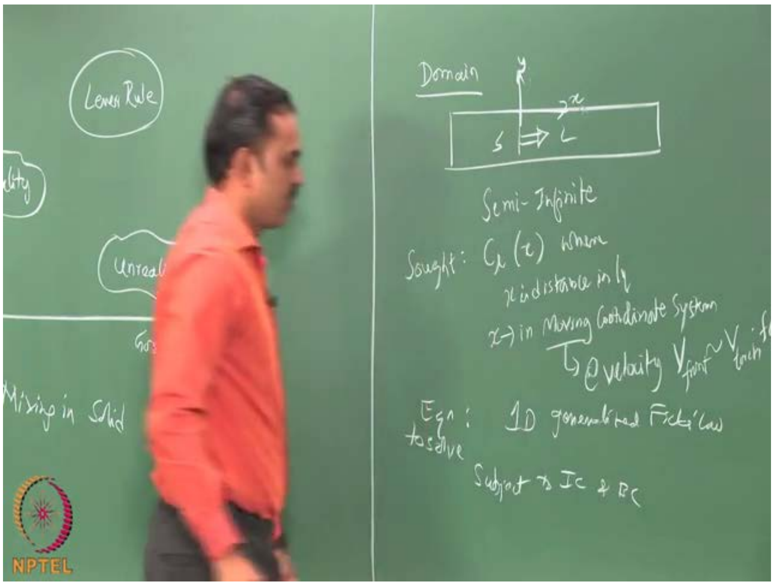

So, the domain we are talking about is like this. This domain size is semi infinite which means that we are taking a particular length, but we are taking that it is. So, large compared to the rate at which the diffusion is going to take place, but it can be considered as semi infinite. And normally, if the diffusion length is L then any domain that is of size 3 L or more it can be taken as semi infinite. So, therefore, this is not something that is abnormal. And we also are going to make some more restrictions on the way we are going to pose his problem we want to actually look at the composition profile only in the liquid.

So, what is sought composition the liquid as a function of distances, where x is the distance in the liquid which means that we want to have a solution in a domain which is actually attached to the interface and is moving; which means that we are actually looking at solute profile in the liquid zone, but as it is solidifying we are only looking at the remaining liquid. So, which means that our distance should be x is in moving coordinate system.

And at what velocity is this interface moving or the coordinate system that we have fixed, so at what velocity it is moving at moving coordinate system which is moving at a velocity given by velocity of the front, and that is related to velocity of the torch through a trigonometric function. Which we can apply for the angle that it is growing with respect to the vertical; and vertical is the direction of the heat source at an angle the solidification is happening. So, in other words, we are actually going to have in a moving coordinate system the equation return and the solutions are going to be applied.

And what would be the equation that we need to solve, equation to solve, it is nothing but the solute segregation model that we have done earlier. It is same equation as we have done, but that is basically 1D generalized Ficks' law which we have already derived or compared with thermal modeling and done, so that is the equation. And it is should be written in a moving coordinate system also and subject to the boundary conditions, the initial conditions and boundary conditions, so that is the problem statement what we have.

And once we have that problem solved, then we do have a grip on how the segregation is going to happen at a micro scale within a small domain that is in the melt pool while it is solidifying. So, we would draw write the equation and draw the boundary conditions right away. Just give me two seconds to erase this part.

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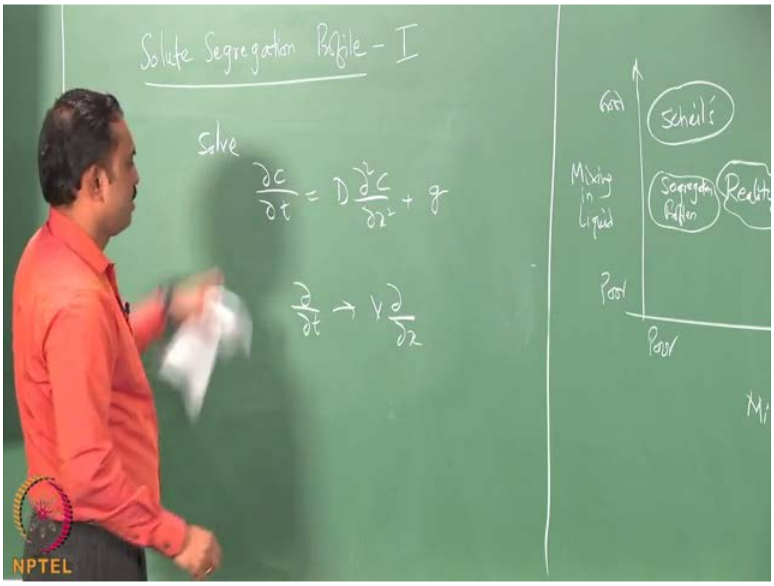

So, the equations we are going to solve this; normally, you would write an equation like this g is the generation term, D is the diffusivity, C is the composition of the solute that you want to solve. And in 1D, this is how the equation is going to be. And we want it to convert the coordinate system to a moving coordinate system, and therefore, that means, the time variable is going to be changed to the distance variable. And the distance is also in the same in x direction which means that this has to be modified.

And we already said that something like this get modified to if the velocity is along x-direction, it is going to be modified like that and therefore, we are going to use that here and change the equation and we would do that.

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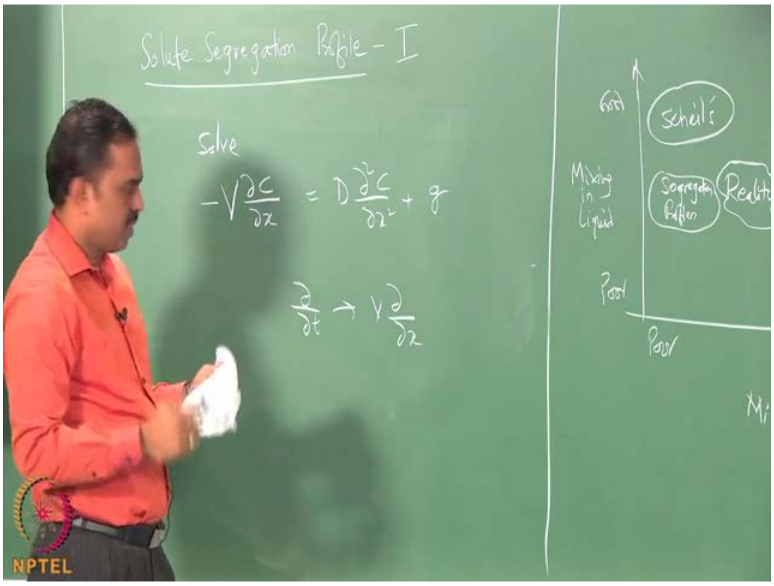

And if you want to sit on the front and see which where the material is moving normally it is moving in the minus x-direction. So, you would put a minus sign. This can be changed depending upon the way you are going to plot. And if x, positive x is going in the forward direction then the velocity which it is the material is moving is in the backward direction if it is on the interface and look. So, therefore, it is going to minus V . So, this is the equation how we are going to do.

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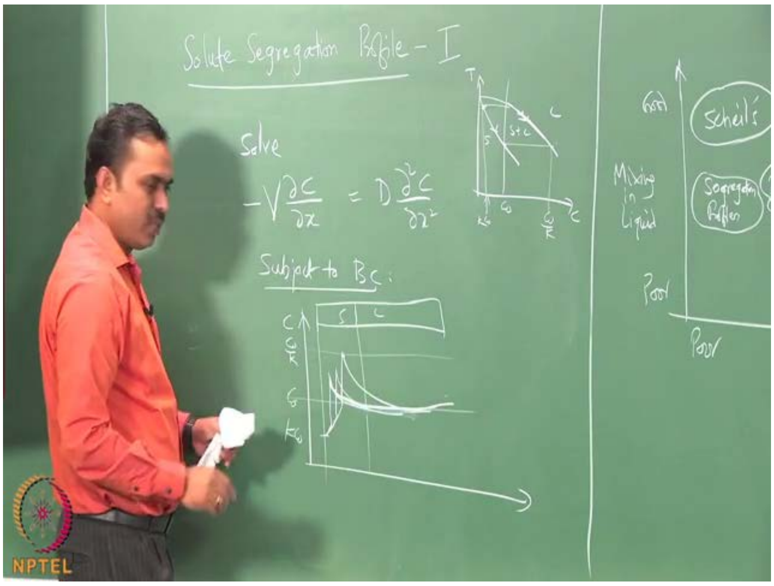

And we are doing it in such a small domain that there is no generation of solute there is no reaction that is happening, so this term can also be ignored. So, in other words, this is the equation that you are going to solve subject to the boundary conditions. And for you to identify what the boundary conditions are then you must at least kinetically draw how the profile is going to evolve. So, that we can actually identify the boundary conditions at x is equal to 0, and at x is equal to infinity. So, for that, I would actually show you how we could draw the profiles schematically and then may the boundary conditions.

If you are to look at from a stationary coordinate system, how this profile of composition is going to be from the solid to liquid as it is moving, then you would notice that if C naught was the composition, initially you will have K C naught and you would see that the composition has go to up.

And you would see that like this, because initial solid to form will be K C naught average composition is C naught everywhere and how much ever solute that is dumped will be in liquid. And then liquid composition is going to be not flat where it is going to be falling in down approaching C naught value as you go far away, so that the diffusion of the solute is happening gradually. And as you keep on solidifying, so this is going to be go up and down. At the point that the solid composition reaches C naught, then the liquid composition should reach C naught by K. This we have already seen from the phase diagram.

Here to recollect I will just draw it here. So, we already have this analogy solid, solid plus liquid, liquid from the phase diagram that if the average composition is C naught then the very first solid that is going to form is K C naught. The last liquid that is going to solidify is C naught by K and they are changing along this path. The liquid composition is going from here to here and the solid composition is going from here to here, so that way we can actually see that the peak is going to be at C naught by K.

Now, there is an argument to say that if the steady state conditions are going to prevail in the moving coordinate system, or in other words, if the profile is going to be stationary profile in the moving coordinate system, then you will have the liquid composition is always at C naught by K and solid composition is always as C naught because these ratio exactly matches the partition coefficient. And you may have a situation where the flux into the liquid due to the diffusion is matching the segregation that is happening.

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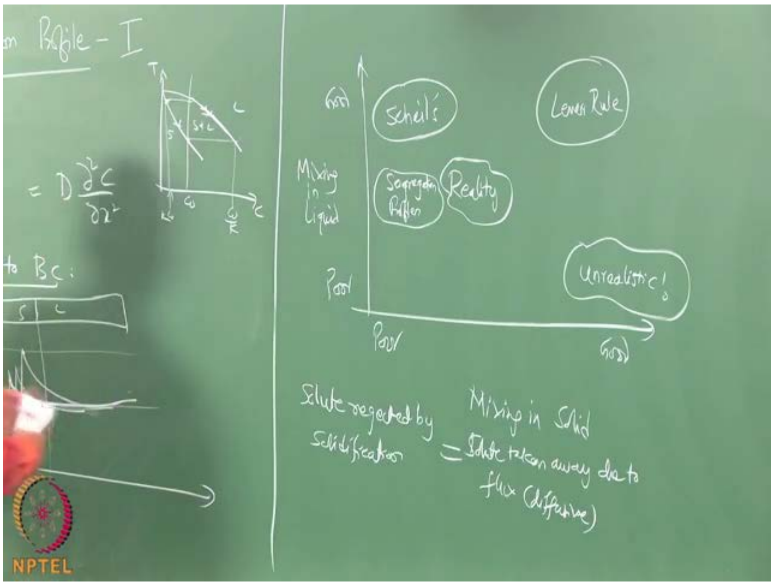

So, under that condition namely when the solute rejected by the solidification is balanced by solute taken away due to the flux - diffusive flux. So, whatever solute is coming into the liquid because of segregation is taken out because of diffusion, and then you have a study state condition possible. Under that situation what happens is that the composition of the solid will be C naught, the liquid composition at the beginning will be C naught by K, and far away it will be C naught.

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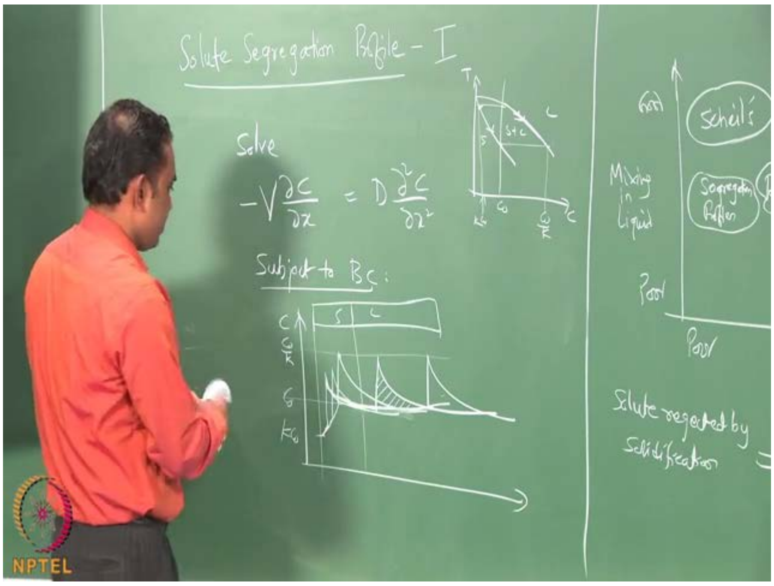

So, how the profile would look after some distances like that and further more. So, it means that this amount of solute that is collected at the interface will be taken along with the interface as you go along and the profile is going to look like this. So, we would then draw that neatly to identify the boundary conditions.

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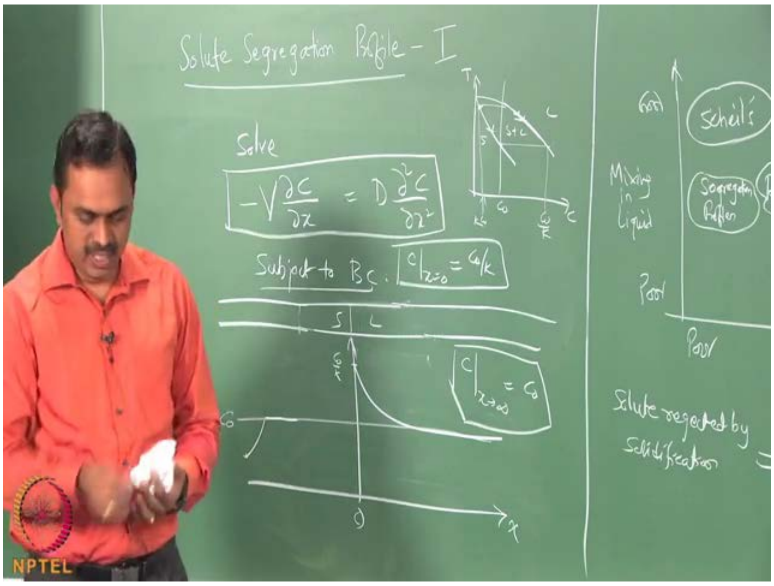

So, let us just do that. So, it means that so as you already we have talked it is a semi infinite domains So, we will just keep that open and this is how it is going to be the composition is going to be overall composition be C naught. And this will be distance; and this value is C naught by K. And somewhere in the beginning of the solute segregation profile, you have a situation of that nature and this is called the initial transient. And for a total length that is several tens or hundreds of the diffusion length scale, this initial transient can be neglected, so that for most of the length you have got a steady state profile.

And if this was the profile then what would be the boundary conditions, we need to inspect if this was the situation then what would be the composition at x is equal to 0, and that will be one boundary condition. You can see that at x is equal to 0; the liquid composition is C naught by K that is one condition. And what would be the boundary condition in the far away, liquid composition at x tends to infinity is C naught, far away it is C naught. So, these two are the boundary conditions we have to apply.

And, this is the equation we are supposed to solve. So, the problem is now completely frozen, solve the diffusion equation in moving coordinate system and 1D without the advection term without the generation term in the liquid subject to boundary conditions.

Where at the interface the composition of the liquid is C naught by K; and far away from the interface it is the same composition as the bulk of the liquid, which is C naught.

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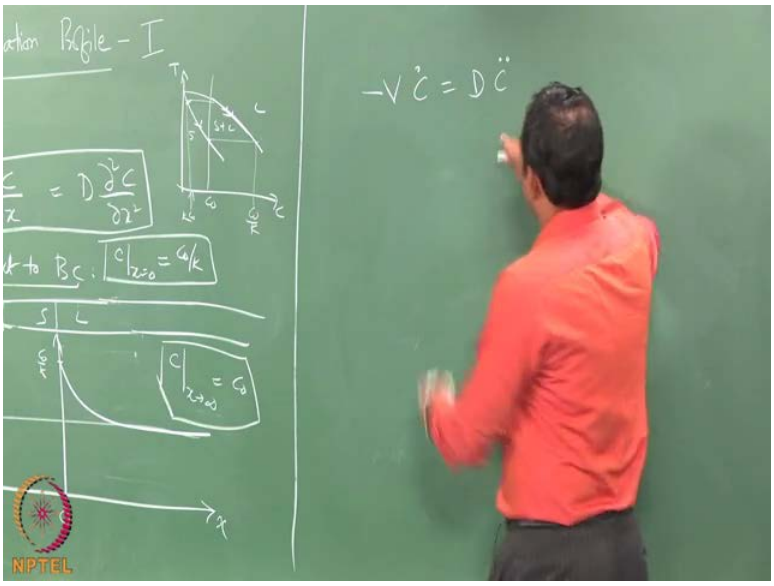

So, we can do that and then we will able to see how this profile will be having a functional form. So, I will do that in a moment. So, let us designate this as C dot is equal to D C double dot. So, dot implies the differentiation with respect to the distances.

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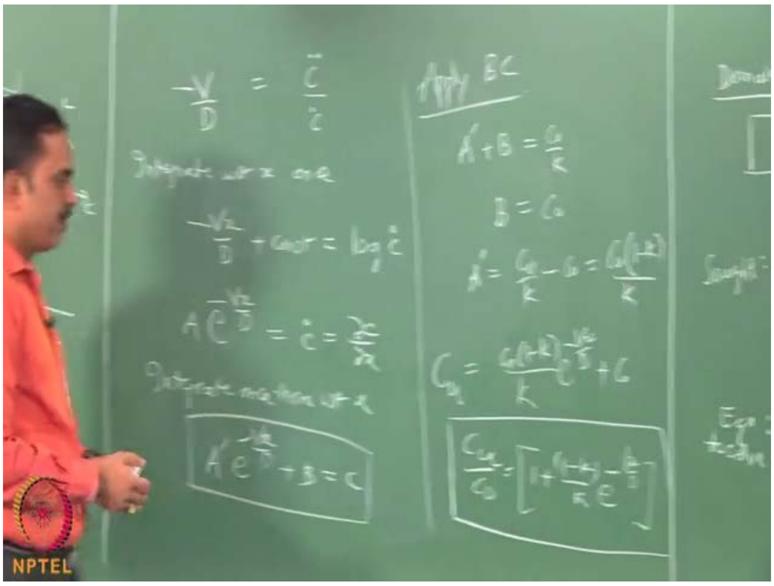

And I will take this fellow down and this fellow on the other side. And we can now see that you have got when you integrate, you have got a variable whose differentiation is on the top and therefore, when you want to integrate, you get the logarithm of it. So, integrate with respect of x once, and you get minus V x by D plus constant is equal to logarithm of C dot. And you can then take the logarithm to the other side, and you can see that it is a exponential, so e raise power of minus V x by d and plus constant will then become a multiplication is equal to C dot which is nothing but dou C by dou x. And then you can integrate once more, and you can see that the integration of e raise power of any function will be the same function, and therefore, it would look like a prime e raise power of minus V x of by d. So, I am just absorbing minus D by V into A, and calling it

A prime and plus constant is equal to C so that is a solution it looks like. The composition of the liquid is going to be B plus a multiplication factor A prime into e raise power of minus v x plus D. Now we can substrate that into the two boundary conditions. You can apply the boundary conditions. And you can see that when you apply the boundary conditions at x is equal to 0, you would see that this one would then go to unity, which means that A prime plus B is equal to C naught by K.

And when you apply the second boundary condition extends to infinity, when extend to infinity this tends to infinity and it the minus sign it goes to the denominator and therefore, it goes to 0. So, it means that B is equal to C naught and that means, that A prime is equal to C naught by K minus B minus C naught; take C naught into common 1 minus K by K. So, you substitute both of these into that equation and you will get the solution as follows; composition the liquid is given by A prime that is this C naught into 1 minus K by K e raise power of minus V x by D plus B, which is C naught.

Now, you can take C naught into the denominator or on the left hand side, so that you can just look at it is a function as follows so that it is like a just a profile. So, you can see that C liquid by C naught is equal to 1 plus 1 minus K by K e raise power of minus V x by D. So, you can see that you have an exponential function to tell you how the composition is varying. When x is equal to 0, then you have got this unity and you can see that it will become basically 1 by K, C naught by K and that is the value C naught by K here. And x is equal to infinity, these goes to zero and that composition will be just C naught and that becomes C naught here. So, we have verified. So, it is an exponentially decaying function is something that we have derived from here.

Now what does it implied to us, it implies that the composition profile in the box towards the weld center is going to be an exponentially decaying function, and that is going to have some implication on how the microstructure is going to evolve. So, we will come to that in a moment; and before we windup, we can just look at this function, and try to simplify some more aspects of it.

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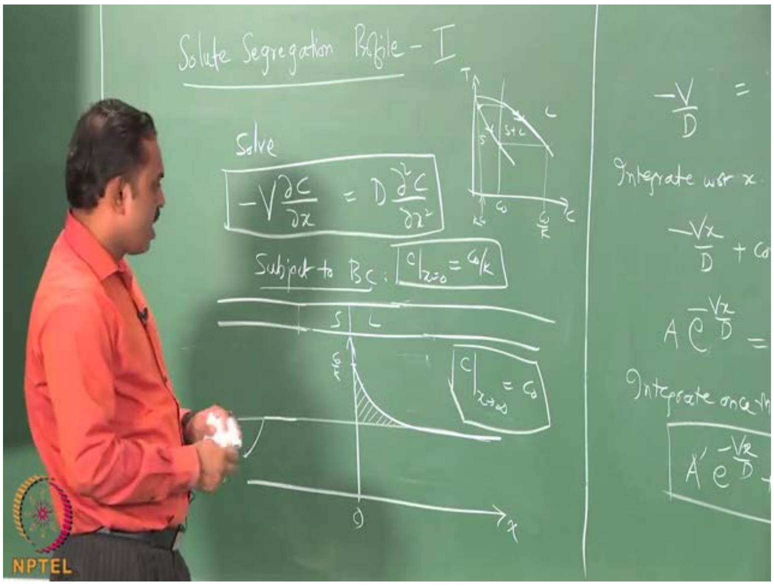

So, the one thing that we want to simplify is as follows can we convert this amount of segregation profile that is there into in equivalent triangle and inspect what would be its width this is something that I would give you as a homework problem.

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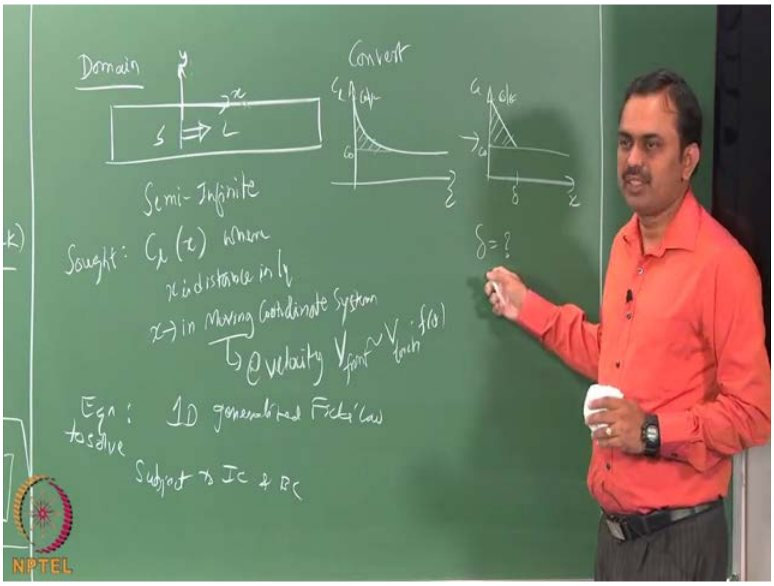

So, the problem itself I am going to state it like this; convert the exponential decaying function into a triangle, whose width is delta everything else is same this value C naught by K, this is C naught, this is C naught by K, this is C naught, so that the areas they are same. And I am asking what would be the delta value. So, we would look at it as a tutorial problem and see how that comes and that would actually tell you what would be the distance over which the segregation is active, and that actually has a very important role in determining how the microstructure of the weldment will be, whether it will be equi-axed or it will be columnar.

And normally, in welding, we would like to have equi-axed microstructure because the impact toughness of the weld joint will be better that way. And what parameter governs that transition, this is one such parameter and we will come to that discussion in a moment.

We will then break at this point and then resume after few minutes to the second parts.