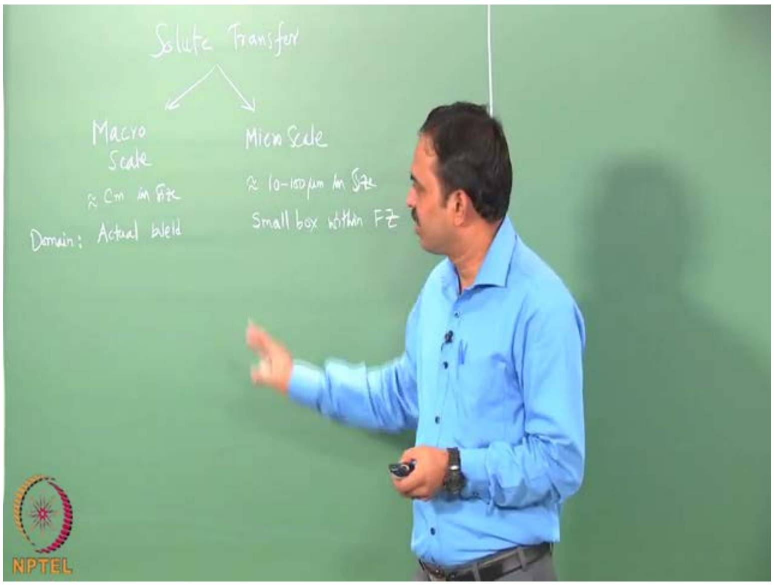
Analysis and Modeling of Welding
Prof. Gandham Phanikumar
Department of Metallurgy and Material Science
Indian Institute of Technology, Madras

Lecture - 13
Solute Transfer Modeling – part 1

Welcome to the lesson on Solute Transfer Modeling. So, in this lesson which will be in several small parts, we will be discussing about the modelling of the solute transfer which is basically the composition distribution and this has to be done at two different lens scales, unlike the thermal or the fluid flow.

The reason being the solute transfer is governed by the diffusion coefficient which is very small compared to let us say thermal diffusivity or momentum diffusivity. So, we will have this lesson divided into two sub-sections as given here.

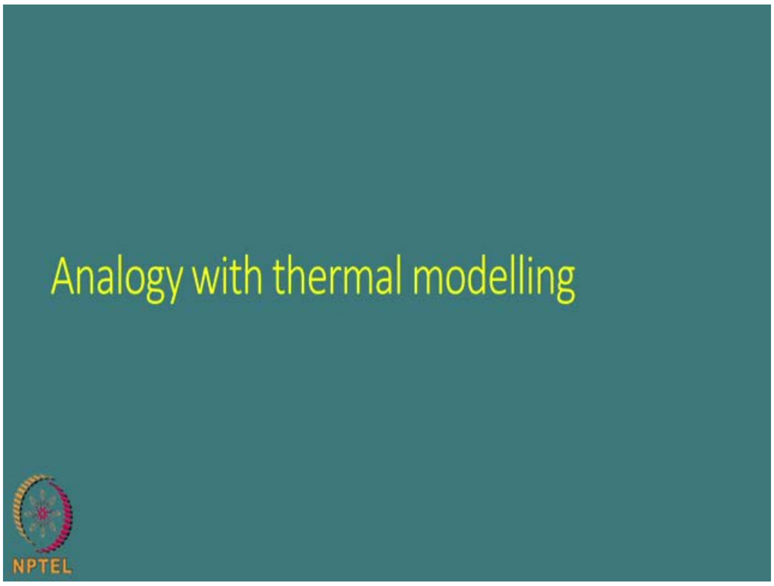
(Refer Slide Time: 00:54)



So, will have it discussed in two parts, the macro scale I will take up first and that will be basically at the system scale which means the domain is nothing, but the actual weld pool itself and you would have the system size in terms of several centimeters depending upon the actual weld geometry.

We also take up later on micro scale model at the same solute transfer, where you will able to see the variation of compositions which are relevant for main certification problem in welding and that could be at a very small scale which is dictated by the diffusive coefficient of the solute in the weldment. And the domain for micro scale model will not be the actual weld, but it will be a small box within the fusion zone and will align the box in such a way that we will able to do 1-D analysis to gain insight into solute transfer. The way we will start with the macro scale model is by making an analogy with the thermal modelling. So, we have already discussed at length.

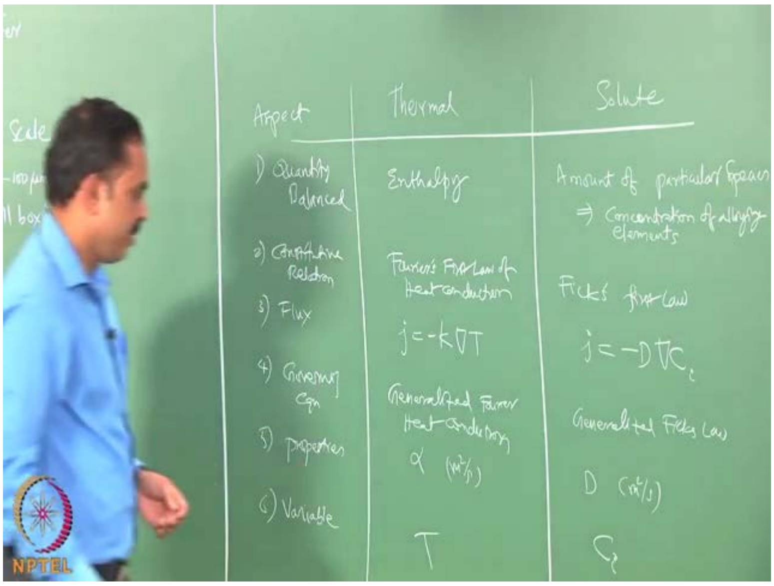
(Refer Slide Time: 01:55)



Analogy with thermal modelling

The thermal modelling way we have derived the equation with a balance and we will be able to then by analogy draw the same kind of a map for various concepts in solute, the transfer also and we will be able to then write the equation by comparing the respective terms. So, let us do that by comparing the various aspects and we will do that map now.

(Refer Slide Time: 02:19)



Aspect	Thermal	Solute
1) Quantity Balanced	Enthalpy	Amount of particular species ⇒ Concentration of alloying elements
2) Constitutive Relation	Fourier's First Law of Heat conduction	Ficks first Law
3) Flux	$j = -k\nabla T$	$j = -D\nabla C_i$
4) Governing eqn	Generalized Fourier Heat conduction	Generalized Ficks Law
5) properties	α (m^2/s)	D (m^2/s)
6) Variable	T	C_i

So, the idea is as follows. In thermal and in solute, we are going compare aspects and we will do it step by step. The first aspect is what is that you are trying to balance in the thermal model as well as in solute model. So, the quantity balanced in this case, it would be the enthalpy and in the case of solute transfer, we are trying to balance the amount of particular species. By species what we mean is basically one of the elements in the case of (Refer Time: 03:13) and sometimes we may also takes species to be ions or compounds, but in our case you would just think of this as concentration of alloying elements. You can say like that because most of the metallic materials, the analysis adequate with just the element.

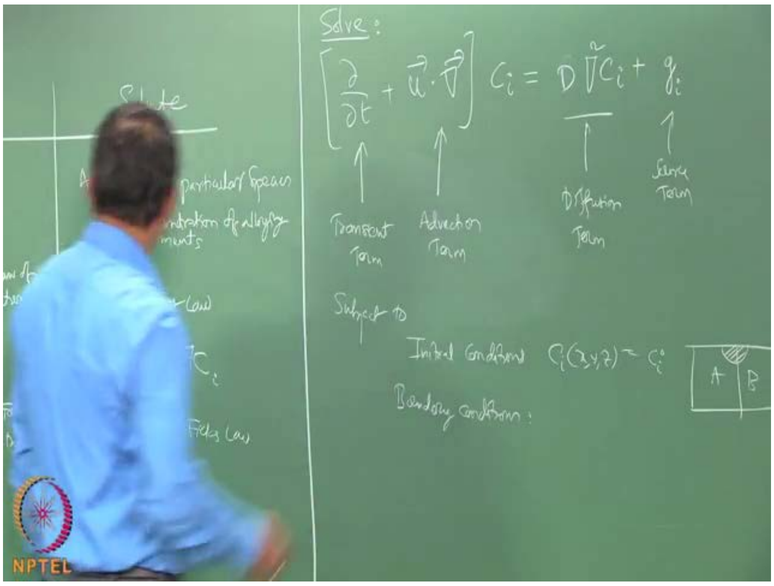
In the thermal model, we have come across what is called a constitutive relationship and that is basically governing cause and effect and that is in our case, we in thermal model we said that it is the Fourier first law of heat conduction. In the case of solute transfer, it would be Ficks first law and how would be expression be for the flux. In case of thermal, we write the flux as j is minus k into grade t, so that the k thermal conductivity grade in terms of temperature giving a rise to a heat flux and in the case of solute, you would write similar expression.

The mass flux is given by minus d into grade of c, where composition of that particular alloying element we are talking about you could actually put I to indicate for what species you are writing this equation and you would have multiple values of d with respect to how many alloying elements are there and for our analysis, we will just take one element in the domain.

What would be further steps, we would see that. You could write the final equation which is basically generalized. So, governing equation is nothing, but generalized Fourier heat conduction equation and in this case, it will be generalized Ficks law. So, in other words, there is one to one mapping for both this phenomenon and therefore, if you look up the lesson on thermal modelling and if you remember the form of the equation, then you could just simply substitute the variables and look at how the equation should look for solute also, and the parameters properties that are playing a role here in this case, it is thermal diffusivity which is in meter square per second that will play a role in this case, it is d diffusivity which is again meter square per second which is playing a role.

What is the variable we are trying to solve the expression is for balance of enthalpy, but then we still want to solve for the temperature as a variable and in this case, we want to solve for the composition of the species that we want to solve for. So, we will then look up the equation for heat transfer and then, simply substitute wherever we are supposed to see t, we substitute c. Where you are supposed to see alpha, you can substitute d and then you should get an equation that should be reasonable for solute transfer also. So, we could write that and then see how it looks like.

(Refer Slide Time: 06:56)



So, here is what I have written the generalized expression and the meaning of the different term as we can relate with the mapping is like this.

(Refer Slide Time: 07:27)

Generalized Ficks Law

This is Generalized Ficks Law and this is not a form that was found to be in many of the books and the form that you would normally see would be this here. I would just put d in

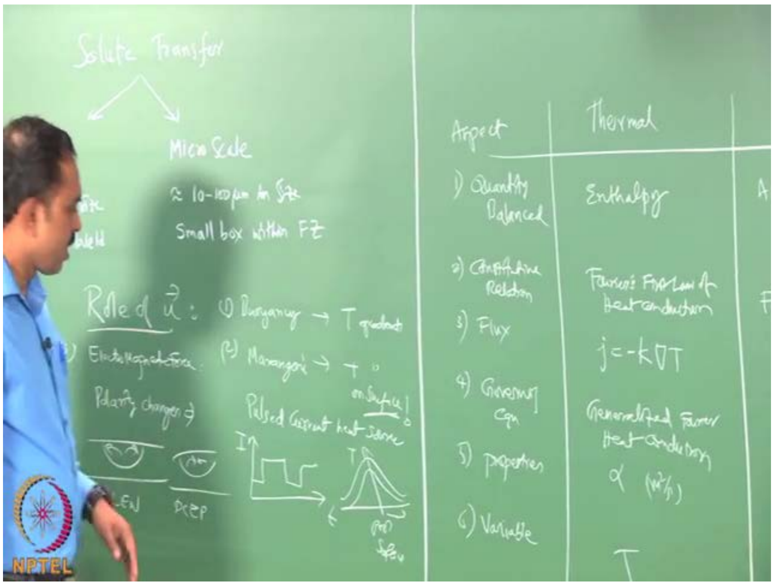
1 d. You would have seen this kind of an expression and I am just making it very general here by writing it not as dow square by dow x square, but with this. So, all that, all three dimensions are taken into account and I am also adding a term which would take the fluid flow into effect and also generation term, so that the analogy with thermal model is complete.

So, in other words, this is not very different from the so-called second law of Ficks D mass diffusion, but it is just a generalized form of the same thing. So, let us just look at the meaning of these different terms. So, this term which you would come as dow c by dow t is the transient term. This is nothing, but the advection term or convection term and this is the diffusion term and this is the source term.

So, if you want to say that, you want to solve for the solute transfer at the macro scale, then what is the problem? The problem statement is as follows. Solve this equation subject to the initial conditions which is nothing, but c i at x y z is known, some initial conditions are known and boundary conditions and we will look at what boundary conditions are applicable shortly and once you have these and the property values and the velocity value etcetera, then basically you have got the problem well stated and that would basically constitute how you want to go ahead with the macro scale solute transfer modelling.

So, the word about the flow and the reason why these kinds of equations are not very popular in the welding literature and why we normally ignore the solute transfer at the macro scale, I would just mention the role of this cause - the velocity here.

(Refer Slide Time: 10:16)



So, you could see that velocity in the weld pool is coming from three different driving forces. The first driving force is buoyancy and it is driven by the temperature gradients causing the density gradients and these do not generally change very much during the welding. However, also the strength of convection is not very high in the buoyancy convection mode.

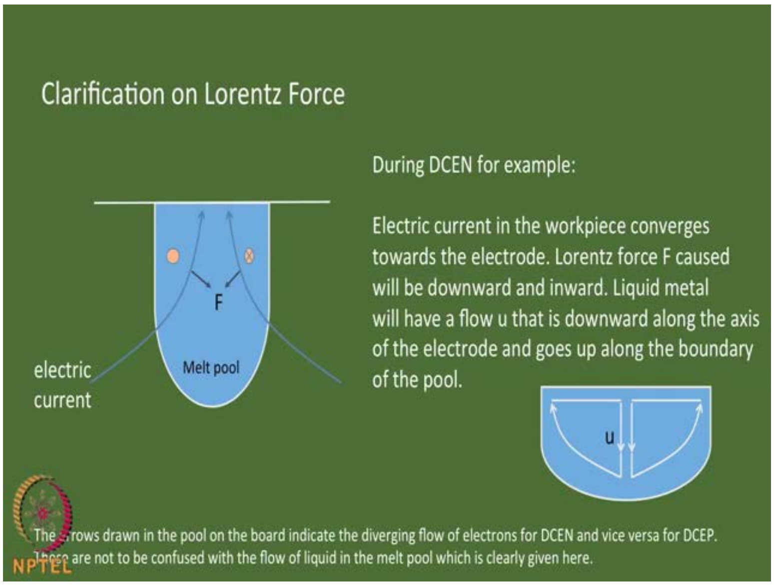
The second driving force would be marangoni and this is also strongly depended upon the temperature gradient on the surface. Now, on the surface would trigger what could happen when we use what is called pulsed current. So, look at what happens if you have a pulsed current heat source or it implies is that and function of time. The current is going to be taking shapes like that and it means that for some duration, the current is high and some duration is low. So, in the durations where the current is high, the maximum temperature achieved will be high and then in the duration when the current is low, the maximum temperature will be low.

In other words, the temperature gradient on the surface of pool if you were to look at that temperature as a distance on the pool surface, you would see that it may fluctuate between two appearances like this sometimes sharp and at sometimes shallow and it can keep fluctuating between these two as of an as the pulsing frequency is going to be there.

So, in other words, the marangoni convection on the very top surface is going to be fluctuating at the frequency that you are going to change the current and any fluctuations implies that the velocity on the surface is going to be fluctuating by that much of change variation that you are thinking.

Now, what is the other driving force which is also going to be important? It is not present in the laser welding, but it is there in all arcs welding. It is basically due to the electromagnetic force. So, here also the same analogy will occur. What happens is that whenever the polarity is changed, you have the AC current used for some of the welding processes. So, whenever there is polarity change are even, the current changes as it is possible in the pulse. So, it would actually mean that the directionality of the convection would be changed.

(Refer Slide Time: 13:12)


Clarification on Lorentz Force

During DCEN for example:

Electric current in the workpiece converges towards the electrode. Lorentz force F caused will be downward and inward. Liquid metal will have a flow u that is downward along the axis of the electrode and goes up along the boundary of the pool.

The arrows drawn in the pool on the board indicate the diverging flow of electrons for DCEN and vice versa for DCEP. These are not to be confused with the flow of liquid in the melt pool which is clearly given here.

So, you may have situations where the current is going away and then, it is coming again inwards as you change the polarity and this would be for example, I am giving you how it would change. Whenever you change the polarity electro negative, electro positive for simple fluid flow situation here which means that as often you change the polarity that often the conduction is going to flip its direction.

So, in other words, this variable u which is coming into the term here is going to be varying very often with the time and is also going to be very strong and we already have mentioned that the diffusivity is very weak in the solutal conditions. That is the solute diffusivity in liquid is very small value compared to the thermal field diffusivity of thermal field, thermal diffusivity. Generally four orders of magnitude are larger than solute diffusivity. So, because of that this is weak and this is very strong and it is also fluctuating.

In other words, the distribution of solute within the domain is governed primarily by the convection pattern and it is going to be well mixed. So, because of that it is usually found that you may not have to solve for the macro scale distribution of mass. Usually it is well mixed, but in case it is well mixed, you could go ahead and do that also.

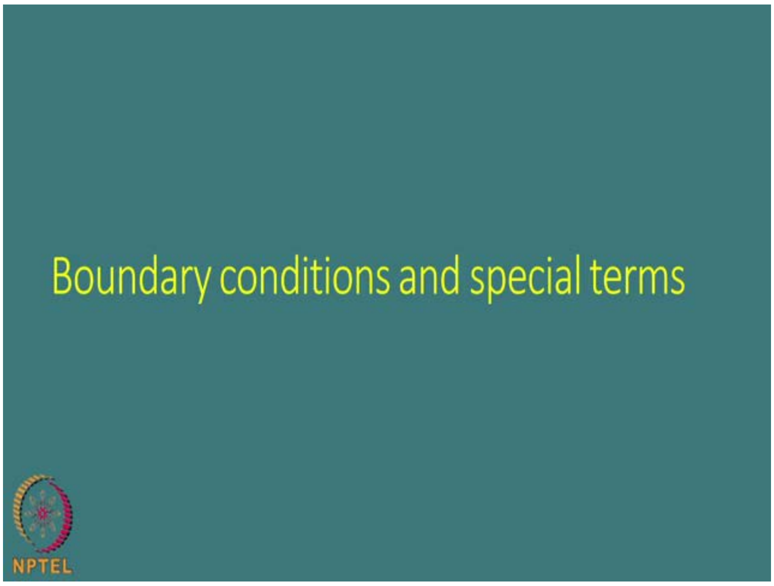
(Refer Slide Time: 14:47)

Initial conditions

For example, if you are using constant polarity and if you are not using pulsing current, surely there will be macro scale grades. That will be grades that will be possible and in such situation solving this may be necessary now one word about initial conditions.

So, initial conditions are basically what initial composition of the material is before you start the welding and this usually means whatever is a composition of the base material, that is going to be the value, that is going to be set and sometimes if you have dissimilar welding, then this value will be two different value on two different halves of the weldment. So, if you have A and B, that is going to be joined. Then you can see that initial value of composition on A side and B side will be different and that is how take into account the dissimilar joining aspect. What would be the boundary conditions? So, the boundary conditions require again some amount of discussion.

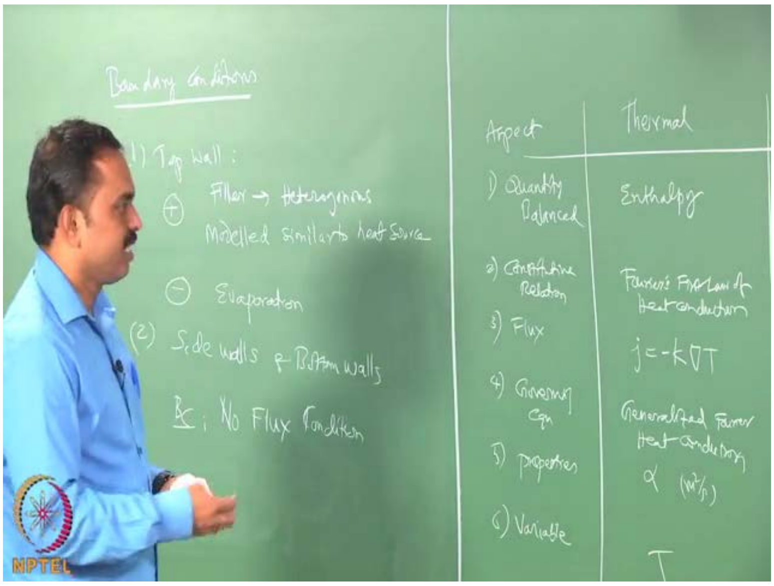
(Refer Slide Time: 15:42)



Boundary conditions and special terms

The boundary conditions are as follows. So, you can go step by step from the top surface to the side walls. Let us look at the boundary conditions for mass transfer.

(Refer Slide Time: 16:09)



Boundary Conditions

1) Top wall :
- (+) Filler → Heterogeneous
  Modelled similar to heat Source
- (−) Evaporation

(2) Side walls & Bottom walls

BC : No Flux Condition

Aspect	Thermal
1) Quantity Balanced	Enthalpy
2) Constitutive Relation	Fourier's First Law of heat conduction
3) Flux	$j = -k \nabla T$
4) Governing eqn	Generalized Fourier Heat Conduction
5) properties	α (m^2/s)
6) Variable	T

So, first is the top wall. So, we should ask a question whether or not there is influx of any alloying element from the top and it would be generally present if there is filler. So, watch out if is filler and if it is inhomogeneous or heterogeneous filler which means that it is different from the base material.

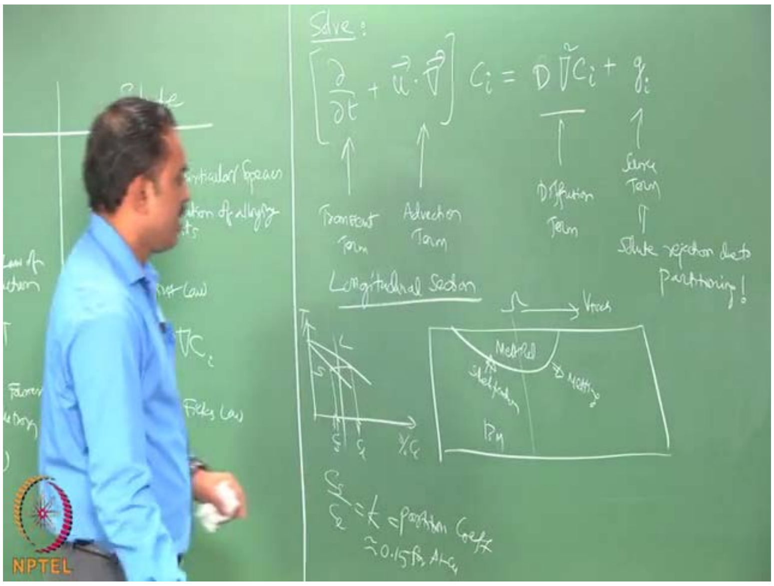
Then, you do have addition of mass from the surface of the pool and that should constitute the mass flux coming in from the top and this can be modelled similar to similar to the heat source because the distribution of these species from the wire is very similar to that of heat also. So, you could have Gaussian distribution coming in from the surface, you may also have top hat that is a uniform distribution solute coming from the top surface and this is when you have addition of material coming from the top.

You also have actually loss of material at the top which is equivalent to the heat loss by radiation and convection. In the case of thermal field, in the case of solutal field, the loss is actually by evaporation. So, evaporation losses are generally found. For example, if you have a welding of 7000 series, you have zinc being lost from the melt pool and such things can also be taken into account and evaporative losses. Then again modelled as heat sinks that are happening and definitely depends upon the surface conditions. So, both kind that is heat sources and heat sinks can be modelled on the top wall.

What about the side walls and bottom? Here the boundary conditions are fairly simple as oppose to in the thermal field. The reason being that the side walls and bottom walls are usually solid and when it is solid, then there is no change in the composition that is happening because as you can see from this illustration if your melt pool is here, then the rest of it is solid and that is not undergoing any change in the composition during the weldment. So, what would happen is if the boundary condition can be written as no flux condition which means that you could write it as equivalent to the adiabatic condition as in the thermal field. So, you could have that kind of boundary conditions that are written.

So, once you have these conditions and the governing equation, then you are set to solve this using any methodology that is available to you. So, numerically or analytically and then, go ahead and do one word about the special terms. So, this source term that is there do we need to have any special term is a question and I would just suggest that we can have it and it will be clear when the module on the micro scale modelling is completed. Let us just look at that briefly if there is any need for a special term. In the case of the heat transfer a thermal modelling, we had a special term which is basically the enthalpy model to take into account late heat evolution. So, analogously here also we will have that requirement that you can actually look at what is called the longitudinal section.

(Refer Slide Time: 20:04)



So, in the longitudinal section, you always capture the vector that is corresponding to the torch and you would have the melt pool and this is the base material and as we have seen earlier on the forward direction, in front of the arc you have the melting that is happening and in the backward, you have the Shelification that happening on the back. Now, what happens when you have shelification at the back is as follows.

If you look at typical simple phase diagram for a dilute alloy temperature and the percent composition, what happens is that the composition of the solid and liquid are not same at any given temperature. They are different and their ratio is also called as partition coefficient which is approximately let say, 0.15 per aluminum copper alloys. So, essentially it means that when a solid is forming out of a liquid, entire composition is not converted as a solid. It will be only a part of it and rest of it has to be left in the liquid itself. So, because of this partitioning effect, then what happens is that on the shelification front some amount of solute will be dumped into the liquid pool and that would have to be taken care as a special condition. So, if you like you could actually take that into the special term or source term here.

So, one possibility is the solute rejection due to partitioning and there are reasons why we normally can ignore that because we have noticed that the scale at which partitioning happening is so small that it could be absorbed within the variations of the micro structure that is possible in the solid as it is growing. So, that at the system scale, really not much of flux is getting dumped into the melt pool.

In other words, the melt pool as it moves along the concentration does not change with time because there are reasons to believe that and that will be evident after we complete the micro scale model of this particular solute transfer. So, at this moment we can say that if at all you want, you could actually the special term to be the solute reaction due to partitioning. Otherwise you can just ignore that term and pretend that the governing equation is having only three terms, namely transient, advection and diffusion term, ok.

So, with that I would say we will close the formulation for macro scale and we will look at some solutions of this particular solute transfer at system scale when we come to the methods of using numerical or analytical based solve this and particularly for dissimilar welding, you do have very interesting solutions possible because the initial conditions are at least rich. So, I will show you some of them in a second part of the macro scale simulation later on. So, we will now then continue on to the part II of the solute transfer modelling which is at the micro scale which means we need to imagine much smaller domain in the weld pool and we will take it up in the next part of the lesson.

Thank you.