

Flow through Porous Media
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Lecture – 27
Miscible Displacement (Step Change in Concentration)

I welcome you to this lecture of Flow through Porous Media. What we discussing was the miscible displacement that is what we are trying to build on in this lecture.

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More importantly we have been talking about this process called dispersion which is diffusion that is mixing inside porous medium when the flow takes place. So, mixing because of flow inside a porous medium that is what we are referring as dispersion and how dispersion takes place in a porous medium that is something which we have been working with. So, what we did so far was we had looked into the dispersion, when dispersion as the flow takes place through a capillary.

So, in this regard we have talked about so called Taylor dispersion. We had we showed that if the velocity profile is uniform; that means, when the front is uniform, when it is almost a plug flow inside the capillary, at that time the diffusion will follow certain equation. On the other hand when there is a velocity profile particularly a laminar flow in a capillary which is the velocity profile, velocity distribution would be parabolic in that

case pulse that you introduce, that pulse will be stretched in the form of a parabolic strip and because of that the diffusion process that the mixing process is completely different.

So, there are I mean what kind of theories that can be what kind of theories would be relevant here we discussed those. Particularly the aim was that the diffusion in a static fluid; I mean if I put drop of ink in a beaker full of water the way the diffusion takes place we try to the retain that same form I mean that is what Taylor has done.

Taylor's dispersion is all about; the Taylor's dispersion equation is all about that they have Taylor has retained that same similar form of the equation and, then compared the what would be the effect I mean when it is a static system I can see, I can feel if I change this parameter this would be the effect. Now, if the same equation form is retained so, if one can extrapolate very quickly and see what would be the impact of various operating parameters when the flow is when there is a non uniform velocity distribution and still mixing is happening. So, all these things we discussed when there is a flow through a tube.

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Diffusion of a step in static system

Diffusion of a concentration front
 Spreading of a front, separating two regions: One occupied by a tracer with diffusion coefficient D initially. Other region is with no tracer initially

Governing Equation remains same as before

$$\frac{\partial c_1}{\partial t} = D \frac{\partial^2 c_1}{\partial z^2}$$

$t = 0, \text{ all } z, c_1 = c_{10}$
 $t > 0, z = 0, c_1 = c_{10}$
 $t > 0, z = \infty, c_1 = c_{10}$

The slide also features a graph of concentration c versus distance z . The initial concentration is c_{10} at $z=0$. As time t increases, the concentration front spreads and the concentration decreases. A red graph on the right shows a sharp peak at $t=0$ that broadens and shifts to the right as time increases.

Next what we are going to do is we have talked about this dispersion when the injected the when the solute is injected in the form of a pulse. That means, what we talked about at that time is that if you have a conduit here and if we introduce a pulse; that means, we approximated it as a Dirac function it is value at t at time t equal to 0, it is value is

infinity at z equal to 0 and away everywhere it is 0. So, this is this is a Dirac function; I mean I this is a Dirac function.

And, then this Dirac function as it travels through these capillary what would be the how these concentration profile how it would be flattened? So, it would be flattened like this because it is it is continuously there is the there is diffusion going on with the upstream and the downstream fluid.

So, that is this broadening we have talked about and we have already put together equations for it under two situations. Under one situation the profile is uniform and in the other situation one has a parabolic velocity profile which we called Taylor dispersion. So, what are the form of equations what are the impacts if radius changes; that means, radius of capillary changes will it be more broadened or will it be more sharp. So, those discussions we had.

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Diffusion of a step in static system

Diffusion of a concentration front

Spreading of a front, separating two regions: One occupied by a tracer with diffusion coefficient D initially. Other region is with no tracers initially

Governing Equation remains same as before

$$\frac{\partial c(z,t)}{\partial t} = D \frac{\partial^2 c(z,t)}{\partial z^2}$$

$t = 0, \text{ all } z, \quad c_1 = c_{10}$
 $t > 0, \quad z = 0, \quad c_1 = c_{10}$
 $t > 0, \quad z = \infty, \quad c_1 = c_{106}$

Smear of front
Cumulative flow

Now, instead of our Dirac function, instead of that if we impose a step change here if we impose a step change in concentration, how we impose a step change in concentration? The concentration was 0 all along or some value all along and then suddenly we had suppose there is a flow taking place and there is a toggle, we have there is a valve which we could turn. So, that the flow is taking place from a different chamber which is than the one we had earlier.

So, here there is a change in concentration; that means, I have two chambers, one was pure water let us say and the other was water with salt or water we dye and then from one chamber there is a switch. Now, it at some time suddenly this concentration changed from 0 to some value and then it continued to flow with that value. So, we continue to flow from that chamber. So, one can implement a step change here at the inlet.

So, how it would come out at the outlet? So, at the outlet we said and in fact, we briefly touched upon this issue that one must ensure that see if we talk about the concentration at the outlet definitely it will be zero for some time because these step change it has to travel all the way through these capillary. So, there is a residence time any fluid that enters into this capillary, there is a residence time after which I expect this to arrive at the outlet.

So, that residence time depends on what is the volume of this capillary and at what flow rate we are injecting this; assuming the entire cross section is participating in the flow. Of course, I mean suppose there is a dead zone inside for some reason that there is a stagnant zone inside for some reason that is not there I mean if we make some assumption that way. So, we can assume that at after you inject this total volume of the; whatever is a volume of this capillary after you inject that much of volume you expect this step change to arrive at the outlet.

So, if we plot concentration versus I can say, I mentioned this before that either you can plot it as time or you can plot this as cumulative flow. So, we mentioned this in the context of pulse. Now, in case of a step change also after this residence time, if there is no stagnant zone entire volume is available for flow, then one can expect that this step change will arrive now.

So, this step change should have arrived here, but fact of the matter is that these step change will not be as sharp as it is because you remember we had a Dirac function and we found it that got broadened, the same thing will happen here also. These step will also there would be diffusion with the downstream fluid, there would be some diffusion. So, so, this because of this diffusion these step change will also be somewhat smeared.

So, this concentration profile would be something like this; instead of a sharp step it would be smeared. So, this is something which we are expecting and so, this is this is this instead of a sharp change we have this smeared front we can call it, smeared front.

And, this smeared front is happening because one has the this diffusion is going on. So, this is this is also a part of dispersion process right only thing is there.

So, the only difference in boundary condition if you look at their these at t equal to 0, you have imposed an Dirac function and instead of that here you are imposing a step change. So, now, if we try to articulate what we are talking about here, diffusion of a concentration front so, we are talking about a step in static system first ok. So, this analysis we are talking about here is basically for static system, not for the flow system. But, our aim is to go to this flow system.

So, first we apply this to the static system. So, what does static system, how do you define it? It is that you have z which starts from z equal to 0 here to z equal to infinity all the way, and the concentration at z equal to 0 is all along held at this concentration c_1 0 ok. So, so initially these entire concentration from z equal to 0 to z equal to infinity these concentration was; let us say this concentration was let us say, so, how do you define here? c_1 infinity. So, let us say this concentration was c_1 infinity.

So, I would say my then these z axis is this is probably the z axis and these value is c_1 infinity and these value is c_1 0. So, from so, for at time t equal to 0 for all z c_1 was equal to c_1 infinity, this is the value. And, then from for t greater than 0 at z equal to 0 c_1 is equal to c_1 0. So, this is what you imposed from for t greater than 0. So, t is equal to 0 this entire domain of z equal to 0 to z equal to infinity entire domain is z concentration c_1 infinity,

Then for t greater than 0 so, moment the counting starts these concentration at z equal to 0 is held at c_1 0 and that is retained that way for all values of t greater than 0. So, because of this one can expect that there would be diffusion from this side to that side. So, that means, one can draw a differential element, one can find out how much would be the flux from left side, how much would be the flux from the right side area perpendicular to the screen is a . So, how much would be the volume of this differential element if we multiply this by the corresponding Δc if there is a change in concentration ΔC .

So, we can draw mass balance how much of mass. So, many kg is entering over duration Δt , how much of kg is leaving from the right phase of this differential element and how much is accumulation. So, we can do that same exercise I had done it in previous

lecture and one can arrive at so called Fick's second law which says that $\frac{\partial c}{\partial t}$, the concentration here in this domain changing with time. So, c is a function of z and t , $\frac{\partial c}{\partial t}$ is equal to $D \frac{\partial^2 c}{\partial z^2}$; c is a function of z and t $\frac{\partial^2 c}{\partial z^2}$.

So, this is the governing equation for a static system, no flow nothing. This was this block was at the concentration c infinity, suddenly moment the time counting starts concentration at z equal to 0 is held at c 0 and from that point on we are trying to track the concentration in these domain, z equal to 0 to z equal to infinity. So, obviously, if we solve this equation I mean intuitively we can see that the concentration will gradually rise. You remember when we had a Dirac function, we found that concentration started rising here right because there was diffusion taking place.

So, here also by the same token there would be diffusion from left to right and because of that the concentration will rise. So, these are the lines, and these are the lines as time increases I have given this by this arrow t with arrow showing upward; that means, as t increases these would be the lines. What is the end of it? At t equal to infinity if you continue you expect this entire domain to be equal to c 0 right. So, that is the endpoint. So, this is slowly this concentration will increase and so, in that case if we try to put these boundary conditions here or initial and boundary conditions the initial condition is at t is equal to 0 for all z c is equal to c infinity. So, at time t equal to 0 everywhere it was c infinity.

Then as time starts t greater than 0 z equal to 0; that means, at this end c is equal to c 0 that is what you are imposing. And then at t greater than 0; that means, when the time started z equal to infinity; that means, far away from these whole things far away from this location where things are happening far away this effect of this will not be felt because our domain is from z equal to 0 and z equal to infinity, not if not a finite domain. So, at z equal to infinity c will remain unchanged. So, z one z equal to infinity c will remain to it is original value c infinity.

So, with these boundary conditions and with these governing equation one can solve and find out what is the concentration, what would be this concentration profile; just like we had a concentration profile I have given you that profile based on similar governing equation, but different set of boundary conditions.

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Diffusion of a step in moving front

Solution

$$\frac{c_1 - c_0}{c_{100} - c_0} = \text{erf}\left(\frac{z}{\sqrt{4Dt}}\right) \checkmark$$

when $c_{100} = 0$, $c_1(z, t) = c_0 \left[1 - \text{erf}\left(\frac{z}{\sqrt{4Dt}}\right) \right]$

The diffusion in negative z will be mirror image, which will reduce $c_1(z, t)$ by half.

Instead of static system, when the front moves at average velocity u , z will be replaced by $(z - ut)$.

Further, when the velocity profile is laminar (parabolic), D is to be replaced by $E_2 \equiv D_{eff} = \frac{R^2 u^2}{48D}$

where R is the radius of the capillary. Aris has shown $D_{eff} = D + \frac{R^2 u^2}{48D}$, when axial diffusion over and above radial diffusion is considered.

Finally $\frac{z}{\sqrt{4D_{eff}t}} = \frac{1}{2} \left[1 - \text{erf}\left(\frac{z - ut}{\sqrt{4D_{eff}t}}\right) \right]$

So, now if you try to solve this equation we have generally the solution can be given as this; this is the solution $c_1(0)$ is the concentration at z equal to 0 which you have imposed; $c_1(\infty)$ is the concentration that was existing at time t equal to 0 everywhere in the entire domain; z is that z distance and divided by $4Dt$.

So, basically this concentration is a function of position time and diffusion coefficient or diffusivity and this is called error function ok. This kind of solution it is a very standard the solution.

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Diffusion of a step in static system

Diffusion of a concentration front

Spreading of a front, separating two regions: One occupied by a tracer with diffusion coefficient D initially. Other region is with no tracers initially

Governing Equation remains same as before

$$\frac{\partial c_1}{\partial t} = D \frac{\partial^2 c_1}{\partial z^2}$$

$t = 0$, all z , $c_1 = c_{100}$

$t > 0$, $z = 0$, $c_1 = c_{10}$

$t > 0$, $z = \infty$, $c_1 = c_{100}$

$\rho \frac{dc_1}{dt} = D \frac{d^2 c_1}{dz^2}$

$c_1 = 0$

$c_1 = \beta e^{\sqrt{\frac{D}{t}} z} + \alpha e^{-\sqrt{\frac{D}{t}} z}$

$c_{10} = (c_{100} - c_{10}) e^{-\frac{z^2}{4Dt}} + c_{10}$

$0 = (c_{10} - c_{100}) \frac{1}{P}$

$c_1' = c_1 - c_{100}$



And, if somebody wants to get to these solution one can think of the very basic steps would be here one can first of all take when you work with these governing equation, first of all one needs to take the Laplace transform. And, the Laplace transform if you take it can be solved by similarity variable also, but if you if somebody you chooses to do this by Laplace transform then it would be $p c_1 \bar{z}$ that is equal to $d^2 c_1 dz^2$ square.

So, this is if you take a Laplace transform of this you will end up with this form and then if you take these, if you solve this or you can write this as $d^2 c_1 \bar{z} dz^2$ minus P by $D c_1 \bar{z}$ that is equal to 0, this could be a way out. And, then you can solve this equation you can write in that case it would be probably better to write this as in fact, since we are not this is true if we assume c_1 infinity to be 0, then probably this is the way it is.

Otherwise it is better to define a deviation variable I mean it is if you are working with c_1 infinity to be 0 that is fine, otherwise I think one I should be talking about some other variables c_1 prime here; this entire thing has to be expressed in terms of a deviation variable so, where c_1 prime is equal to c_1 minus c_1 infinity. So, one has to define a deviation variable and then it is; and this is the transform variable is I am putting it in as a bar. So, this is c_1 prime bar. So, this would be equation here and if you solve these you one can get c_1 prime bar is equal to it would be that the solution would be a $1 e$ to the power $m x$ plus a $2 e$ to the power minus $m x$.

So, that means, let us say I put a constant $B_1 e$ to the power square root of P by $D z$ plus $B_2 e$ to the power minus square root of P by D into z . So, in that case one can have if this is the solution then one thing is noted at this point that at z is equal to infinity. At z equal to infinity c_1 is finite, but here in this case if you put this as infinity this will not be finite. So, the only way you can make this finite is by holding this B_1 as 0 ok.

So, when you put use this boundary condition so, automatically B_1 would be equal to 0 and B_2 would be simply equal to $c_1 0$ prime bar; prime means making it a deviation variable instead of calling it $c_1 0$ you are writing $c_1 0$ minus c_1 infinity and bar means you are taking the this is the transformed variable. So, once you write this and on top of that one can write this $c_1 0$ prime bar one can if you look at the true definition of

Laplace transform that is equal to $\int_0^{\infty} c^{-1} e^{-py} dy$ that is a definition of Laplace transform.

And, if you now take $c^{-1} 0$ and $c^{-1} \infty$ these are constant. So, if you take this out $c^{-1} 0$ minus $c^{-1} \infty$ and then if you do this integration of e^{-py} from 0 to infinity these would be simply $1/p$. So, in that case you can write in that case you can write c^{-1} prime bar that is equal to $1/p$ $c^{-1} \infty$ $e^{-\sqrt{p} z}$. So, that becomes the concentration profile if you follow the Laplace transform.

And, then if you go to the table for Laplace transform and go to the and take the inverse Laplace transform, so, then automatically the equation that I mentioned will simply follow; that means, in that case you will be ending up with so called c^{-1} prime would be equal to $c^{-1} 0$ minus $c^{-1} \infty$ into $1 - \text{erf}(z/\sqrt{Dt})$ actually this is this should be P they does not matter because it is it is a limit to the integral it can be $pt dt$.

So, it is error for this should be t and this should be here $t^{-1/2} \text{erf}(z/\sqrt{Dt})$ divided by $2\sqrt{Dt}$. So, this is after you take inverse Laplace transform you get this quantity and this c^{-1} prime is once again is equal to c^{-1} prime is a deviation variable. So, it is $c^{-1} 0$ minus $c^{-1} \infty$.

So, this could be the chain of thoughts one can get to ok. So, this is a very standard equation with this kind of bound this type of boundary condition and these solution in terms of error function is very common. And, one needs to know this that is a error function if you look at this if the type the error function the way error function plot is if somebody plots a error function of x as a function of x , it is generally it remains linear from 0 0 it goes all the way linear up to 0.65 – 0.7 around that and then it starts curving out and the idea is that error function of 1 the limit would be 1.0 asymptotically it reaches 1.0 as x tends to infinity.

Similarly, on the negative side error function of minus x would be minus of error function of x . And here also it will follow the similar trend and asymptotically reaching minus one as x tends to minus infinity. So, this is a error function typical behavior of error function.

So, now this is; now that we know this let us look at the solution once again. So, this was the solution we have $c_1 - c_1^0$ by $c_1 - c_1^0$ equal to error function of z divided by square root of $4 dt$. So, this gives me under in static system what would be the concentration profile; that means, I have given a step change. So, I see that the concentration gradually rising as time progresses. So, as time progresses as time increases concentration is gradually rising and it will this concentration at any point at any z at any time it would be it will be following this equation.

So, when $c_1 - c_1^0$ is equal to 0; that means, truly I mean earlier we had held these as $c_1 - c_1^0$ and these as $c_1 - c_1^0$ right. So, when this is truly, this is $c_1 - c_1^0$. So, that means, it is going all the way to zero. Then, we can simplify this further, then $c_1 - c_1^0$ becomes equal to $c_1 - c_1^0$ into 1 minus error function of this quantity.

Now, one thing you must note here; now, suppose there the gradually what do you would do is we have this is what is happening in the static system. So, what next we will do is; we will take this up to the flow system. Flow system obviously, if we are working with a plug flow we can say that we have to go for a moving coordinate system as we had done earlier.

That time we had z^2 , so, instead of z^2 I am talking about for the pulse for the Dirac function there or until a dispersion everywhere we had written we had e to the power z^2 term right. So, in that z^2 we had to write it as $z - \bar{u} t$ whole square right when we had a uniform velocity and when we have these it was v naught the average velocity in case of a Taylor dispersion. So, we had to go for a moving coordinate system; that means, we assume that this whole thing that we have here, here it is a static system now as if this step is moving in z .

So, that is why we had to go for a moving coordinate system that is one thing that we must note. And, second thing is when you give a step change in concentration and then you expect this to travel or step change with time would be then this is with space. So, step change with time would be this. So, as this concentration step change travels we said that, we have only looked into this part of the concentration assuming $c_1 - c_1^0$ to be fixed, but when you implement a step change $c_1 - c_1^0$ will not be fixed.

$c_1 - c_1^0$ will also because I am not maintaining $c_1 - c_1^0$ here. Something is diffusing out from here, moment something is diffusing out from here means here also some loss would be

there parallelly. This side you have a gain and you are assuming there is no loss from this side $c_1 = 0$ is maintained. So, that will not happen when you put a step change because something is being; something is travelling to the, something is diffusing into the downstream side means there is a loss in the upstream side. So, that also has to be accounted.

So, this is something which we would be addressing in the next class and we will continue. So, keep this in mind that we have to now all the understanding of static process that we have to extend it to a flow system. And, in the flow system obviously, there will be a moving coordinate number 1, number 2 in the as we have assumed in static systems $c_1 = 0$ is maintained it as fixed, but that is not possible in a flow system because anything, any gain on the downstream side has to be there has to be an equivalent loss in the upstream side, that also has to be accounted.

So, these are the things we will discuss in the next lecture module. So, this is all I have as far as this particular module is concerned.

Thank you very much.