

Microscale Transport Process
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Lecture No. #10
Mixing

I welcome you all to this lecture of Microscale transport process. What we have been discussing so far is various microfabrication techniques. We have discussed how to fabricate, discussed about how to fabricate a channel on a silicon or glass wafer, and how to cover that channel with a lid using an anodic bonder or a fusion bonder. And also we discussed various techniques to fabricate plastic microfluidic devices, and we discussed about various advantages and disadvantages of these devices. So, so far what we have and of course, we have discussed about how to put a tubular, how to put, how to insert a capillary, so that this microstructure device can be interfaced with the external world. So, we pretty much we have already done with various microfabrication techniques.

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Biocompatibility - material response

- Generated by the device inside host tissue.
- Caused by diffusion of body-fluid from host tissue into the device.
- Device material swells, develops micro-cracks on the surface → altered mechanical properties, and in some cases leaching.



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What the last issue that I am left with as far as the microfabrication is concerned is biocompatibility. Many of these microfluidic devices, they will be used in they are supposed to be used in human body for various reasons, either to analyze, either to release drug at some point or analyze the level of toxins or due to various reasons, you need it needs to be put human body. So, the major part of microfluid, major part of the applications of microfluidic devices covering human body. So, we need to understand some issues here or at least the terms here that are important. A biocompatibility, we hear this term so often, these material is biocompatible that mean if you insert in human body, you do not expect a adverse reaction; that is the immediate response that I will get, if I ask you this question, what a biocompatibility would be.

Now, the way this biocompatibility is defined here is in this slide I write, biocompatibility there are two points here; one is called material response and the other is called cellular response. One is the response that is given by the material itself; that means, you insert a microstructure device inside human body. Now that material will respond in certain way, I mean you have to ensure that the material remains intact; the material does not erode or the material does not swell, so that is important. The other issue is the cellular response, the cells around that material, the human body that should not get destroyed.

So, there are two points here, one is that microstructure device should not get destroyed by human body, because human itself contains lot of chemicals and if that microstructure device swells, ruptures, erodes; so, if that does not function then the purpose would be lost that is one issue. The other issue is that the material that you insert in human body that should not cause some adverse reaction that the cells around that material gets destroyed, then you have some other problem. So, if we get back to this material response, material response is generated by the device inside host tissue. So, this material response is generated by the device, not by the human body, it is by the device that you insert.

And this is caused by diffusion of body fluid from host tissue into the device. Diffusion of body fluid, the body fluid is there and you have inserted these material inside human body. So, this material is coming in contact with the body fluids. Now, if the body fluid diffuses into the human, diffuses into the, diffuses into this device and then that device material swells, that is a third point that I write here; device material swells, develops

micro cracks on the surface; altered mechanical properties and in some cases leaching,so these are the problems that would happen.

If this, if the body fluid enters into the device and because of that the device material swells, it develops micro crack. Swelling involves, I mean the moment it starts swelling, I mean you never you do not know what is going to happen, because you are stretching it someplace it is getting stretch, someplace it is not. So, there would be stretches developed and at any point there could be a crack developing. So, swelling as I mean something which you have to be careful with develop, so develop some micro cracks on the surface and it can have altered mechanical properties. If something swells, it has to have some kind of structural integrity and that integrity would be lost, so that is a problem with the material.

And in some cases, there could be leaching; that means, the body fluid may leach out some essential part of that device. Suppose on the device, you have some coating and the body fluid starts leaching, you know what a leaching is; so far you have in various chemical engineering applications, you understand what leaching process is. If you have not, I suggest you read any mass transfer book, say mass transfer by Coulson and Richardson or mass transfer by Treybal, you can pick up any of the any of these books in the library and then you can read these chapter leaching.


It is like you this body fluid will take away some material from the surface of that microstructure device. So, then if such leaching happens, then a microstructure device will lose its structural integrity, it will lose its ability to perform inside human body; so, these are not wanted basically. So, this is what I refer as material response. So, this is as far as the device part is concerned. The other part is the cellular response. Once you put the device, you have to ensure that the cells around it should not get destroyed, the body cells that are around is device that should not get destroyed. So this cellular response, this is generated by the host tissue.

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Biocompatibility - cellular response

- Generated by the host tissue.
- Inflammation at the device-tissue interface, reddening and pain. If the inflammation lasts long and damages local cells → device is cytotoxic.
- Otherwise, chemical signals released by the damaged tissue attract white blood cells.
- A fibrous encapsulation made of foreign body giant cells and macrophages is formed around the device.
- If the encapsulation does not affect the functioning of the device → **BIOCOMPATIBLE**.

Tests: *In vitro* (in laboratory glasswares) and *in vivo* (in live animal or human).



So, this is generated by the host tissue, inflammation at the device tissue interface. So, moment you put this microstructure device, there would be inflammation at the device tissue interface, these will cause reddening and pain. If the inflammation lasts long and damages local cells that is referred as, then the device is called cytotoxic. I mean, one thing I would like to point out at this point out here is that moment you insert a material, external material in human body, there will be inflammation, there will be reddening, there will be pain; so, these are few things which will happen invariably. And if these things happen that does not necessarily mean that the body is that the, that microstructure device is not biocompatible.

You cannot say that, because anything you put this will invariably happen, but what is important here is whether that thing dies down or not. Whether the inflammation is after sometime the inflammation goes away, after sometime the pain goes away, then only you will take that material as biocompatible, it is as straight as this. So, inflammation at the device tissue interface that will happen, invariably whether it is biocompatible or not biocompatible. This reddening and pain, all these things will happen, but these will not last long, that is the indication of a biocompatible material. If it lasts long, and damages it starts damaging local cells, then the material is not biocompatible; then the material is referred as cytotoxic, then the device is referred as cytotoxic.

On the other hand, chemical signals released by the damage tissue attract white blood cells. I mean typically, if we material which is supposed to be biocompatible, what will happen is immediately there will be inflammation, because a moment you put external material inside human body, the body will react in certain way, that is a must. If it does not happen, then it is not doing its job. So moment it happens, moment you insert a material inside human body, then there would be chemical signals released by the damage tissue. Some tissue will be damaged, otherwise you will, you cannot because it is an integrated, it is an intact tissue.

Inside that moment you are putting a material; that means you are damaging some tissue some portion you are cutting out. So, those damage tissues they will release some chemical signals and that chemical signal will ensure that white blood cells get attracted to that place. Basically, it is a human body sense that portion of body sends (()) to rest of the body that why there is a problem here. So immediately this there would be signals and blood cells, this white blood cells getting attracted. And in due course, a fibrous encapsulation made of foreign body giant cell and macrophages is formed around the device; that means, this white blood cells that get attracted, it form a fibrous encapsulation made of foreign body giant cells and macrophages, this is formed around the device.

So, if this fibrous encapsulation forms; that means, you are still okay, you do not problem; the material is, it is destroying the cells rather what it has done is, the portion the tissue that you have damaged intentionally, when you put the device inside, those tissues they send a signal and attracted white blood cells, which forms an encapsulation around the material. So that part is still the material can be biocompatible as a matter of fact I mean, I heard people who has I heard of people, who have bullet inside the body and they living, they are just they said that it is too troublesome, you have operate and take out the bullet, so let it be there.

So let it be there means it has already formed a fibrous, there is a fibrous encapsulation around that bullet and it is just safe, I mean there is no more fallout of that injury, so that is what is what I am referring to here. A fibrous encapsulation made of foreign body giant cells and macrophage is formed around the device. Now, one problem could be that these encapsulation that you have, these encapsulation may not allow the device to function properly; that means, suppose it is this device is a controlled release device.

Controlled release device means when you want it will release some drug at a specific location and when you do not want the drug will not be released; so that is the purpose of the device. Suppose the device that you have inserted. Now, if you have encapsulation made, and that encapsulation does not allow the material to release the drug, I mean it is drug is release, but it cannot permit through that encapsulation, then the purpose is lost. So, if the encapsulation does not affect that is the point I have here, if the encapsulation does not affect the functioning of the device, then you call it biocompatible, I wrote it in uppercase here in the slide; that then this is called then this encapsulation then this device is called biocompatible.

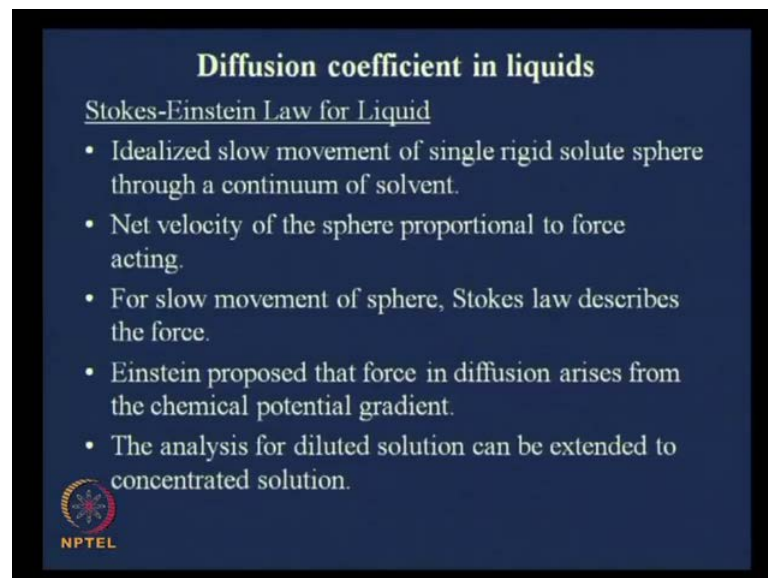
So, you have many checks. First of all, it should not be cytotoxic. First point, if it starts destroying the cells no way, you cannot take it that is cytotoxic, so it is left out. Then it come, then it may come that it is not destroying, but it is forming a fibrous encapsulation and that is disturbing the performance of that device, then again you have a problem. But if that does not even that does not happen, then you can consider this material to be biocompatible; so, this is how you define biocompatibility, I mean in simple term.

Maybe there are other issues involved, as far as this course is concerned I thought this two slides on biocompatibility would be important, at least you have this in mind that anything that if that is inserted in human body and it starts inflammation or pain that does not mean that the material is not biocompatible. It could be that it is just simply biocompatible, because any material you insert in you human body, this will end up with inflammation, pain, reddening, and all this, but this should subside this should not continue for long. Now, there are various tests done to check, whether the material is biocompatible or not.

There are two types of tests, one is called In vitro test. In vitro, vitro you know where the origin of this word vitro, see In vitro means in laboratory glassware and In vivo, that means, in live animal or human. So first, suppose you have you can probably do some kind of screening by In vitro test. And then, once you have identified, once you shortlisted few items, these are items I can considered to be considered them to be biocompatible, then you can run it on some animals, whom you can scarifies, for example, rat. So that is one that is how it is done.

And once you know that it is not going to affect at least some animal body, then you will go for human trial. So, these are the ways biocompatibility is tested. So, this is one important tissue biocompatibility and these microstructure devices, they are very often used in human body for various reasons. So, one could be release controlled release of drug, other could be say there could be glucose monitor placed inside the human body, it is continuously its measuring the level of, if the patient is diabetic, it can continuously monitor his health. So, there could be such devices inserted into human body. So, these are basically some sensor so which would sense how the body is performing. Or it could be the material which can release drugs in a controlled manner. Or it could be simply mechanical it gives some mechanical action like pacemaker or materials like this. So, these are the, so these are issues of biocompatibility that we must know as far as this course is concerned.


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Diffusion coefficient in liquids

Stokes-Einstein Law for Liquid

- Idealized slow movement of single rigid solute sphere through a continuum of solvent.
- Net velocity of the sphere proportional to force acting.
- For slow movement of sphere, Stokes law describes the force.
- Einstein proposed that force in diffusion arises from the chemical potential gradient.
- The analysis for diluted solution can be extended to concentrated solution.

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Now, this probably this ends the discussion on microfabrication, what are you do is, I will probably come back to this later, if any such problem comes up if my if we need revisit this microfabrication issue. What I want to get in now is basically the theories of microfabricated devices; I mean the transport processes which we have, our original intent was to study the transport process in microscale and that now we are getting into this. But I thought this background of how this microfabrication is done, will give a very good idea about how things are done in practice.

Instead, I mean you can always do it in theories, but first you would know where the limitations are as far as implementing things in practice; then probably your understanding would be much better, I mean what we do with theories.

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$h \approx 100 \mu\text{m}$
 $U = 1 \text{ cm/s}$
 $D \approx \frac{2h}{\pi} \approx \frac{2 \times 100 \mu\text{m}}{\pi} \approx 64 \mu\text{m}$
 $\left. \begin{matrix} 10^{-5} \text{ cm}^2/\text{s} \\ 10^{-9} \text{ cm}^2/\text{s} \end{matrix} \right\}$

$\frac{\mu}{\rho} \approx 10^{-5} \text{ cm}^2/\text{s}$
 $\text{Re No.} \approx 1$

$\text{Knudsen Number} = \frac{\lambda}{D_h} = \frac{k_B T}{\sqrt{2} n m^2 P D_h}$

$k_B = \text{Boltzmann const.} = 1.38066 \times 10^{-23} \text{ J/K}$
 $T = \text{Temp. in absolute scale}$
 $P = \text{Pressure}$
 $\sigma_m = \text{molecular diameter of the diffusing species.}$
 $D_h = \text{hydraulic diameter.}$

$100 \text{ cm} - 1000 \text{ cm.}$
 $\lambda \rightarrow \text{Å (liquids)}$
 $\lambda \rightarrow \mu\text{m (gases)}$
 $\frac{\text{liquids}}{D_h} \approx \text{nm}$

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Now, when it comes to the theories, what I would like to introduce first is, one thing you have to keep in mind that suppose the dimension of microchannel is say 100 micrometer. And you have μ by ρ , this is say I should write say channel somewhere close to 100 micrometer and μ by ρ is closed to 10 to the power minus 5 centimeter square per second. I mean you can check, what is the viscosity of common material that you have, what is the density you have? And you will see probably, we come here μ by ρ is around 10 to the power minus 5 centimeter square per second.

And then, if we considered a velocity of one centimeter per second, I mean which is reasonable I mean think of I mean we are talking about a microstructure device which we are going to insert in human body. So, velocity of one centimeter per second would be considered pretty high that in that respect, one centimeter per second we are talking about. So, if we use these parameters and you somebody checks what is the Reynolds number. You will find that even with the higher level of velocity your Reynolds number come, this Reynolds number comes closed to one. Reynolds number closed to one, I mean I have studied fluid mechanics we are we talked about thousand is the transition.

So, Reynolds number of one is practically at the lower end of laminar flow; even I mean you can say laminar flow, even at the lower end of laminar flow; so that where we are operating, when it comes to the flow in a microstructure device. So, when we remember in earlier classes, we talked about these fluid flow fractionation and we are using these, if the concept of laminar flow one layer sliding against the other and then diffusion is taking place from one layer to the other; these I mean we know for sure that we are nowhere close to turbulence.

We know for sure that then one layer is moving and then the other layer is gently sliding against the other, because we are really at the low end of laminar flow. So that is one thing you need to keep in mind that generally we operate around this Reynolds number 2, 10, not more than that. The other point here is that you have this diffusivity, diffusivity is of the order of, diffusivity can be defined as penetration of the, penetration for species divide the distance by which a species penetrates square of that divided by the time. Time it takes for the species to go up to that distance. That is how we commonly understand diffusivity or diffusion coefficient.

The distance that it has look at the unit of diffusivity, it is centimeter square per second. So, this is typically what we understand about diffusivity; a molecule diffusing means it will penetrate up to distance Δx in time t , then Δx^2 by t is typically the diffusion coefficient. Now, if that is so, then you can write suppose I have a channel, I have a certain length of a channel, suppose I have a channel I have half of it is a solute stream going in and half of it is I mean a stream which does not have a solute and they are flowing side by side. And I expect them to mix, when it comes when it comes out. If one layer is flowing against the other, if one layer is sliding against the other, then you can expect that there would be diffusion taking place from one layer to the other.

So, if one stream has the solute; that means, solute means I am talking about say salt solution; if you have salt solution and if you have pure water and if you put them together side by side, you expect salt to go into the other stream which is pure water and when you extract, when you take the entire solution at the outlet, you should expect that the entire stream would be well mixed; that means, the portion which was pure water is now salty. So, that is that is the diffusion we are referring to.

Now, if we expect that over the length L , if the length of this channel is L , the dimension of this channel is say h , if the half width of this channel is h say if the half width of this channel is h and you have the velocity as u , you have the velocity as u . In that case, you can expect, just think about the diffusivity. What is the diffusivity you have, 10^{-5} to the power minus 5 centimeter square per second that is the typical diffusion coefficient you have. For a common say NaCl solution if you have, then that is the common diffusivity. Now, if you put this diffusivity and if you expect this Δx , that is the penetration. Now that it has to penetrate by entire half width, at the end of the channel, then only you can consider them to be well mixed.

So, if that has to happen, what should be the length? Because, you can write t as, so this t can be written as L/u ; that is the time taken for this fluid to reach the outlet. So, that is the time taken for the fluid to reach this outlet. And at the outlet, the penetration should be complete; that means, this Δx^2 should be replaced by h^2 . If you use these parameters, what you will find is that, now the diffusivity can be say I am assuming 10^{-7} to the power minus 7 centimeter square per second, it could go all the way up to 10^{-5} to the power minus 5 centimeter square per second; if we are talking about diffusion of hemoglobin. Instead of sodium chloride solution, I mean sodium chloride is just a hypothetical one; nobody will mix water and NaCl in a microstructure device.

Now, one can mix hemoglobin that he can do. So, if you are talking about diffusion of hemoglobin, we are getting into 10^{-7} to the power minus 7 centimeter square per second. So, if this is the range of diffusivity I have to cover and if somebody asks you, what should be the length of this channel? If this is the fact, this h you know this is a typical dimension of a microchannel is 100 micrometer. So what would be the length we are talking about here and you will find that this length varies from 10 centimeter to 1000 centimeter; if this is the range diffusivity that has to be covered. So, it seems this diffusion is not is the slow process, I means it is it will take.

So, if you expect two streams flowing side by side and it will have complete mixing at the outlet, the length of the channel should be 10 to 1000 centimeter; 1000 centimeter means we are talking about 10 meter. Typically, human height is 1.6, 1.7 meter. So 10 meter, I mean we are talking about that kind of length. So, we are not in definitely in a microchannel this is not a microstructure device. So, you cannot accomplish such level of mixing using two streams flowing side by side and relying entirely on diffusion.

So, you have to have some other mechanism going on, which by which what you do is you increase the interfacial area; that means, the two streams they are flowing side by side, if you introduce. So, called say probably in (---) it would be baffles. If you introduce baffles, by which you introduce extra area, interfacial area over which the mass exchange can take place; then probably you do not need such a long channel. So, my point I mean why I introduce this diffusivity? I mean the two issues that I point out here, first of all the Reynolds number is really small in this case, we have already pointed out it would be around one.

And second point is that if it comes to mixing of two streams in a channel, you cannot expect them to flow side by side and get mixed. You have to introduce some baffles or some other method to arrange the mixing. And that some other method is introducing baffles, introducing some amount of chaos in this mixing process. So, but you got to understand here is by putting baffles, when we put baffles, one idea of putting baffles is to create some amount of turbulence. So that around the baffles there would be AD's forming, I mean in a conventional sense in a pipe, when you put baffles, you will make you will start having AD's.

AD's means packets of fluid flowing from one end to the other, which is in transfer to the actual principle flow direction. So, these are and that is that is associated with turbulence. And in this microfluidic device, we are nowhere close to turbulence; we are in the low end of laminar flow. So, by putting baffles, the idea here is to create additional interfacial area. That the two streams, one is the solute stream, another is the solvent stream, they should have larger area for mass exchange. So, for that you introduce baffles. So that the purposes little different, we will discuss this, we will put the theories of what is, we call this chaotic mixing; this mix by putting baffles and arranging a mixing, this mixing is referred as chaotic mixing.

Now, this chaos is different from the chaos that is referred in context of turbulence, because nowhere it is turbulence. But this chaos is some I mean we will get it to the theories of it probably by the end of this class or may be in the next class. There is third issue, there are three issues I would like to point out, one is the issue of Reynolds number I said, another issue is the length that if you rely on diffusivity alone, then it would be a very long channel, which we cannot afford.

The third issue is there is something called a Knudsen number, which is defined as λ divided by D_h . and what is λ ? λ is the mean free path of the molecule, which can be written as $\frac{k_B T}{\sqrt{2} \pi \sigma^2 p}$ and this whole thing divided by D_h . D_h is, I mean hydraulic diameter, you can say or some kind of characteristic dimension of the channel. So, one is the mean free path and the other is the hydraulic diameter. Now, for now what are the various things, I have here $k_B T$, etcetera; I mean you know what that is, k_B is basically Boltzmann constant, the value would be 1.38066×10^{-23} joule per K. T as temperature in absolute scale.

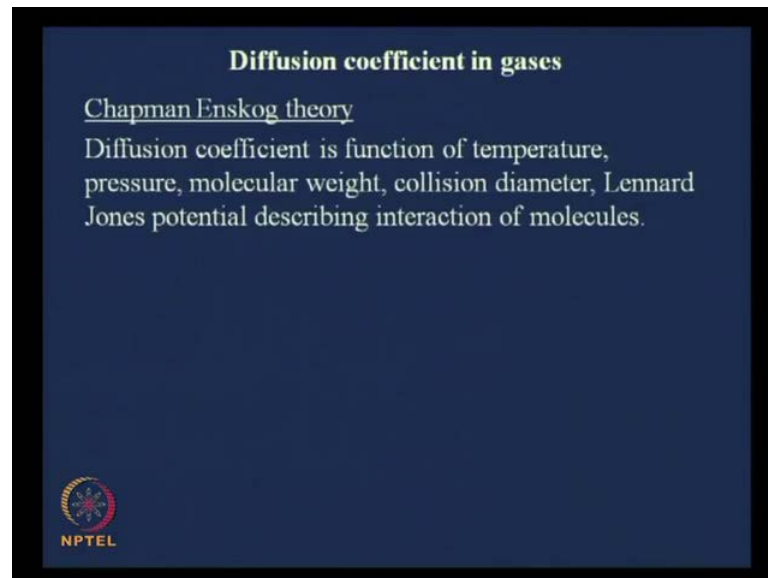
Then you have P , which is pressure and you have σ , which is molecular diameter of the diffusing species; and I said D_h is the hydraulic diameter. Now, if you look at the values of this λ , if you look at the value of values of this λ , in case of a gas and in case of a liquid; for liquid, it is of the level of angstrom and this is of the level of micrometer for gases. So, what is what we conclude from here? If you have λ as, λ in the order of angstrom and λ is of the order of micrometer in case of gases, then the Knudsen number would be important for what which material; it would be for a gas. For the gases, the Knudsen number would be important, I mean see we are talking about this D_h .

If the Knudsen number will be important for liquids, Knudsen number will be important for liquids, if the D_h is of the order of nanometer. For liquids, if the D_h is of the order of nanometer, then you can consider the Knudsen number to be important. But that is not probably that does not come under the preview of this microscale process. Possibly, if you are working with a separation process, where you were separating some molecules within the liquid, then probably you would be working with that kind of range. But for a microstructure device, I mean our, we at the very at the very outset, we said the channel dimension is 100 micrometer. So that for the, that kind of size the Knudsen number is not important for liquids.

For gases, Knudsen number has some relevance; in fact, it is of the order of micrometer, so for gases you need to consider the Knudsen number. Now, when it comes to a mixing, generally the mixing we referred to the mixing of liquids, because mixing of gases is much easier; because diffusivity of gases will be much higher. So, mixing we are referring to is mixing of liquids.

So, here in this context knudsen number is not important. So, these are some of the issues that we should have in mind. Now, when it comes to the definition of diffusion coefficient D , these are available in various handbooks, the diffusivity of various materials. But if I get into the theories of it, I see that there are two established theories, which define diffusion coefficient for liquid and for gas.

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For gases, this goes by the name Chapman-Enskog theory and for liquids; it is Stokes-Einstein law for liquid. These, you can refer any standard textbook on transport process; it need not have to be a microscale, because diffusion coefficient is a very general topic. So, transport phenomena by Bird, Stewart, and Lightfoot that would be just, I mean they have a very good discussion on this Chapman-Enskog theory as well as this Stokes-Einstein law. Briefly, I point out what we have here in Stokes-Einstein law, here we have the assumption here is about idealized slow movement of single rigid solute sphere, through a continuum of solvent. So, while deriving this theory, they have assumed slow movement of single rigid solute sphere; sphere through a continuum of solvent.

Through a continuum of solvent, solid rigid solute sphere is moving, idealized slow movement. Net velocity of the sphere is proportional to force acting that is what the assumption there is. For slow movement of sphere, Stokes law describes the force and there has to be a driving force here. I mean you are treating the diffusing species as a rigid sphere and that is moving through the continuum of solvent.

What is the driving force? Where is the force? I mean why to move, the force is basically arising from chemical potential gradient, that is Einstein's proposal here. The mean for a rigid sphere in a continuum, what would be the force, what would be the drag acting on it that is already defined from fluid mechanics. Now, in case of a diffusing species, there was not any force, I mean I am not pushing the molecule like a, I mean I am not using an external force to push the molecule. So, the driving force here is basically the chemical potential gradient, because diffusion happens, because you know why a diffusion takes place; because of a concentration gradient and the other of concentration gradient is probably the chemical potential gradient. And then, this analysis can be extended for first analysis was done for diluted solution and then it can be extended to concentrated solution.

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Force = $6\pi\eta R_0 v_1 = -\nabla\mu_1$

η = viscosity of liquid
 R_0 = radius of diffusing species

$\mu_1 = \mu_1^0 + k_B T \ln \pi_1$
 $= \mu_1^0 + k_B T \ln \frac{c_1}{c_1 + c_2}$

c_1 = solute concⁿ
 c_2 = solvent concⁿ

When $c_1 \ll c_2$

$\nabla\mu_1 = \frac{k_B T}{c_1} \nabla c_1$

Flux = $v_1 c_1 = -\frac{k_B T}{6\pi\eta R_0} \nabla c_1$

If I write these Stokes law here, the Stokes law states that force is equal to $6\pi\eta R_0$ into v_1 . What are these now, π is 3.14; η is the viscosity of liquid, R_0 is the radius of diffusing species and v_1 is the velocity. This is originally; this equation is available where these formula was available for a drag force. Suppose, if you have a rigid sphere and you have fluid flowing like this, the drag force exerted on the solid that can be given by this formula; where v_1 is the velocity of this sphere. So, the drag force is defined by this $6\pi\eta R_0 v_1$.

Now, this is the proposal of the proposal here is that this is equated with the chemical potential gradient. Now, what is chemical potential for dilute solutions? Chemical potential is defined as some reference plus that same Boltzmann constant temperature and \ln of x_1 . x_1 is nothing but C_1 by $C_1 + C_2$, where C_1 is equal to solute concentration and C_2 is equal to solvent concentration. So, when C_1 is much less than C_2 , you can write μ_1 is equal to, from this expression, you can write $K_B T \ln C_1$.


And the flux by in the context of mass transfer, the flux is equal to $v_1 C_1$, solute concentration and the velocity of that solid of that rigid sphere; so that is equal to $v_1 C_1$, so you can write this as $\frac{-K_B T}{6 \pi \eta R_0} \frac{dC_1}{dx}$, because you are invoking this formula here. So, flux can be defined as this and you know what a flux definition of flux is; flux is d into $\frac{dC_1}{dx}$. So, from this you can conclude that this could be the diffusivity of the liquid. So, this is how, I mean if it is completely an unknown material. So, for a dilute solution, you can find a diffusivity. Now, for concentrated solution, there are correction factors which are introduced.

So, the analysis for dilute solution that is a last line in the slide can be extended to concentrated solution. So, if nothing is there in your hand, probably you can use a formula which already people have already the scientists and researches they have already proposed. In case of gas there is this Chapman-Enskog theory, where diffusion coefficient is written as a function of temperature, pressure, molecular weight, collision diameter, Lennard-Jones potential describing interaction of molecules. You can as I said you can refer Bird Stewart Lightfoot and find the exact formula there. I mean, I just here sitting here, I can point out that you can find these diffusivity values in hand books tabulated or you can use some established theory, at least you can go close to that; if not exact, because the measurements are far more exact than these theories. These theories are based on certain assumptions and models; however, these could be handy, if you do not have any place to start with.

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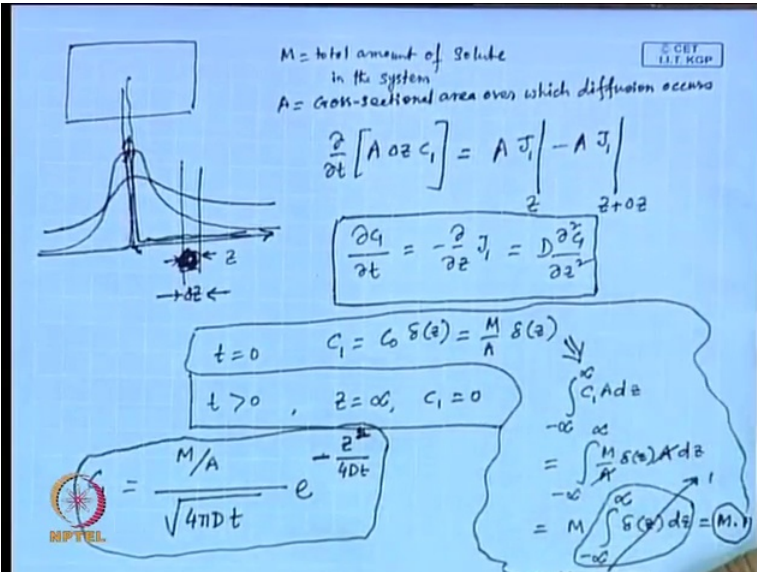
Spreading of a spot in a resting fluid

- Very small spot of tracer at $t = 0$ is expressed using Dirac function that is zero everywhere except at the origin.
- The integral of the Dirac function is equal to one.
- Mass balance on a differential volume.
- Boundary conditions
- Concentration = $f(z, t)$



The next topic, I consider here in this discussion is the spreading of a spot in a resting fluid. See, I mean my idea here is that we have to characterize this mixing, we should be able to theorize, how this mixing will take place in microchannel geometry, if you introduce baffles, if you introduce more said artifacts in the microchannel. But first you need to understand, how the diffusion takes place in a simple situation. So, we first try to find out what all equations we need to consider, if we need to find, if we need to describe spreading of a spot in a resting fluid.

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$M = \text{total amount of solute in the system}$
 $A = \text{cross-sectional area over which diffusion occurs}$


$$\frac{\partial}{\partial t} [A \partial z c_1] = A J_z \Big|_z - A J_z \Big|_{z+\partial z}$$

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

$t = 0 \quad c_1 = c_0 \delta(z) = \frac{M}{A} \delta(z)$
 $t > 0, \quad z = \pm \infty, \quad c_1 = 0$

$$c_1 = \frac{M/A}{\sqrt{4\pi Dt}} e^{-\frac{z^2}{4Dt}}$$

$\int_{-\infty}^{\infty} c_1 A dz = \int_{-\infty}^{\infty} \frac{M}{A} \delta(z) A dz = M$



Spreading of a spot in a resting fluid means this is a resting fluid, a beaker full of water, and then you put a spot a minuscule drop of a dye ink; and then immediately you see the color diffusing into this resting fluid. How will you theorize this, what kind of theory will describe this spreading of color. So, a very small spot of tracer at t equal to 0 is expressed, how will you express a very small spot of tracer. Let us see intuitively, what do we see; intuitively, if we try to find out; suppose, we are treating this as a one-dimensional problem. So, if it is one-dimensional problem, suppose this is z and this is the concentration; you plot the concentration as a function of z .

So, at t equal to 0 what is the condition? At the beginning, it is a spot of tracer. So, spot of tracer, a very small of spot tracer at t equal to 0 that can be expressed using a Dirac function. The Dirac function is zero everywhere except at the origin; so, origin is this point. So, to start with you have profile, which looks like this. So, it is zero everywhere except at the origin. Now what the, what these the other thing that has to be satisfied here is that suppose you put, say M is equal to the total amount of solute, total amount of solute in the system **M is equal to total amount of solute in the system.**

Now, this total amount of solute in the system has to be conserved, by that what I mean is if I look at say at higher time at t equal to 0, I said it is zero, everywhere except at z is equal to zero; it has a finite it has some value. And the integral of this area under this curve, I mean the area under this curve that has to remain same, because as time progresses how would be the profile. This is travelling all the way up little higher time like this, some more higher at a further time instant, it would be like this; and gradually, it would all flat end up.

Now, the area under this curve that should remain same and that should correspond to the total amount of solute in the system. Now, whether you consider Dirac, I mean so the Dirac function has to take care of this aspect. That area under this curve even if you have a Dirac function, if even if you have zero everywhere except at the origin, the area under that curve as well has to correspond to this total amount of solute in the system. So, the area under the curve remain same, because you are not importing any solute from outside; that is that original spot which is spreading out. So, the integral of the Dirac function is equal to one; that is because that has to otherwise these you cannot satisfy this total amount solute in the system, so that has to be satisfied.

Now, if you write the mass balance **if you write the mass balance** on a differential volume. How that be? you would be writing, here suppose you pick up, at some distance z , you pick up a differential length dz or say Δz . Let us say Δz ; we let us develop this from scratch. So, you are picking up a distance Δz . So, you would be what you would be writing at, if you are drawing a mass balance there, you would be writing $\frac{d}{dt} (A \Delta z C_1)$ that is equal to $A J_1$ that is a flux at z minus, the flux at $z + \Delta z$. What is A ? A is equal to cross-sectional area over which diffusion occurs. So, this is the mass balance on this differential element and then if you write this as $\frac{dC_1}{dt}$, then this would be equal to $-\frac{d}{dz} J_1$, which can be written as $D \frac{d^2 C_1}{dz^2}$.

So, this is the governing equation. I mean you are familiar already, familiar with this governing equation, you must have seen this equation in the context of mass transfer. Only we revisit that and we ensure that for **((C))** part of tracer that we arrive at this equation. Now, one thing you must understand that this C_1 would be written as $C_1 = \frac{M}{A \Delta z}$ that is equal to M by $A \Delta z$. So that is the condition at $t = 0$. And at t greater than zero, only thing we know is that at $z = \infty$ $C_1 = 0$ that is the other condition we have. So, at $t = 0$ concentration follows the Dirac function that is the idea of Dirac function.

And what is essentially what does this mean? This means that integration between minus infinity to plus infinity; so, it is zero everywhere except at the origin. So, what that mean see $\int_{-\infty}^{\infty} C_1 A dz$, that would be equal to integration minus infinity to plus infinity M by $A \Delta z$. And A , A cancels out, M comes out of the integral, so A cancels out M comes out of the integral. So, basically this is $M \int_{-\infty}^{\infty} \delta(z) dz$ and I pointed out this that integral of this Dirac function is equal to 1; so that is what I am I said that it is this is equal to M into 1. So, this is basically M .

So, material this result is M , because this integral the value of this integral is equal to 1. So, that is what probably I referred here in this slide as the integral of this Dirac function, basically I should have said from minus infinity to plus infinity. So, this is basically the condition that we have. So, one condition is at $t = 0$. We satisfy this, but that is what we have, in hand the other condition is at $t > 0$, $z = \infty$ this $C_1 = 0$. Because add $z = \infty$ that is far away from the

spot, from far away from the place where you put this spot of tracer, there is no effect.

That is what you say here the C_1 is equal to 0. That means, the color cannot go all the way to the infinity, because after all you have put a very small spot of tracer. So, these are the two boundary conditions and this is the governing equation. Now, this equation there is a solution existing. So, what may be done is, we will we can I can give you the solution right way, so that you can get, I mean when you go back you keep this in mind how it looks. And probably, in the next class, we will briefly touch upon, basically you need to use the Laplace transform to solve this equation.

However, this handling this Dirac function handling, this boundary condition will not be straightforward, there is a trick to it; this particular boundary condition in Laplace transform. You try to do it, after you go back, after this class, you try to do it yourself, I give you the final form. The final form is M by A square root of $4\pi D t e$ to the power minus z square divided by $4D t$; this is the final form z square mind it, z square by $4D t$, this is the final form that we have. So, when you go back after this class, you try to see if how it can be solved. In fact, the next problem that will be picked up is where you do not have a spot tracer, rather you have a front.

Suppose you have a front, that means, you have concentration which is all the way here. So, your boundary condition would be different at that time. This would be z is equal to 0 you have C_1 as C_0 , that kind of boundary condition. They are probably handling this boundary condition is much easier, but here this it is not straightforward. What you what I suggest you do is you go back and try to solve this using Laplace transform. And next class, we will probably spend first couple of minutes to find out what are the intermediate steps. So, thank you all, that is all for today.