Introductory Mathematical Methods for Biologists
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Lecture – 28
Diffusion Constant and Einstein Relation 1905

Hi. Welcome to this lecture on mathematical methods. We have been discussing diffusion and we talked about the diffusion constant and the current due to the concentration difference today our topic is understanding diffusion constant.

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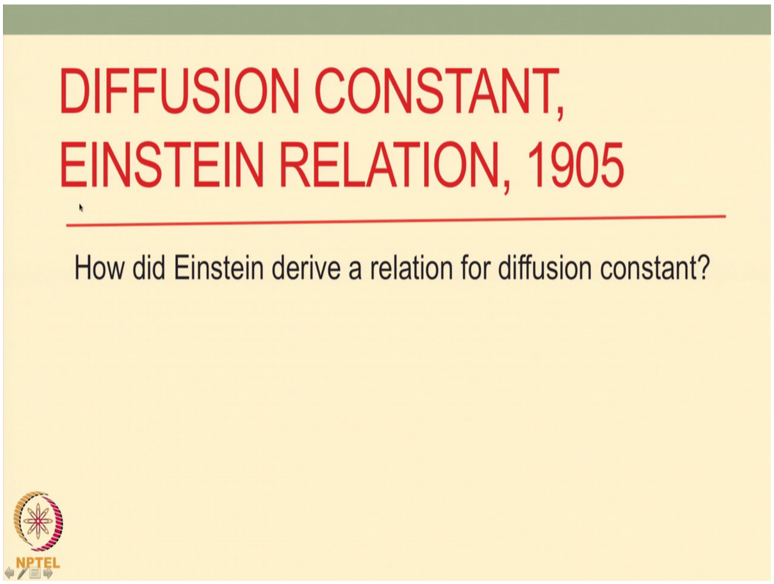

The topic is diffusion constant, Einstein relation 1905 and the question we will answer is how did Einstein derive a relation for diffusion constant.

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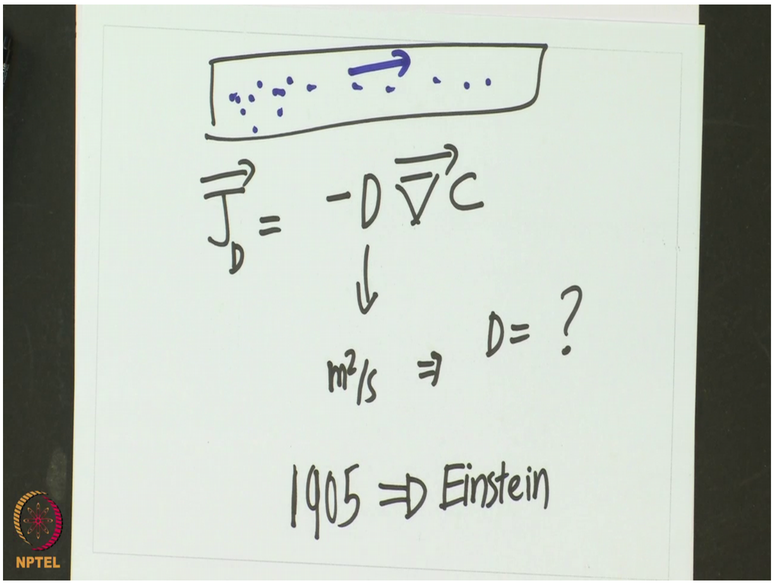

So, the thing that we learnt which is the D which was a part of this equation which is the current or the flow of proteins due to diffusion when you have a when you have a cell or a tube having a constant and a high concentration at one end and a low concentration here.

There will be a flow in this direction and this flow J this is a diffusive flow due to diffusion is minus D del C. So, this is something that we said and we find out the dimension of D or the unit is meter square per second, but what all D depends on what is D? What are the things that D will depend on; the diffusion constant will depend on. So, this is a question that Einstein try to answer in a very famous paper in 1905; 1905 Einstein's paper Einstein.

So, some of you would know that Einstein wrote many famous papers; in the year 1905 is called a miraculous year because one person produce so much work in that one year. So, in that miraculous year, he also wrote a paper on the Brownian motion. So, what is Brownian motion? Brownian motion is essentially diffusion of particles or it is related to the diffusion. Diffusion is related to the Brownian motion. So, because of the temperature since the temperature is 300 Kelvin; around 300 Kelvin in biological system in the room temperature is around 300 Kelvin the water molecules in every in water in the cell; for example, would be doing a zigzag motion and because of that they will go and hit the proteins and the proteins will move around they will jiggle around.

And this would lead to some kind of random motion and this is the basis of diffusive motion. So, base using idea from statistical physics kinetic theory Einstein thought about this and derived a relation for diffusion constant D. So, we would see how Einstein derived it is so simple that it is application of the calculus that we learn. So, far if we apply that we would get the ideas we learnt so far; if we apply we could get; we could get some idea about how Einstein got this relation for D it is. So, we will see that how this was obtained in the in this lecture.

So, let us think about this. So, for that let us consider the following case where we have container.

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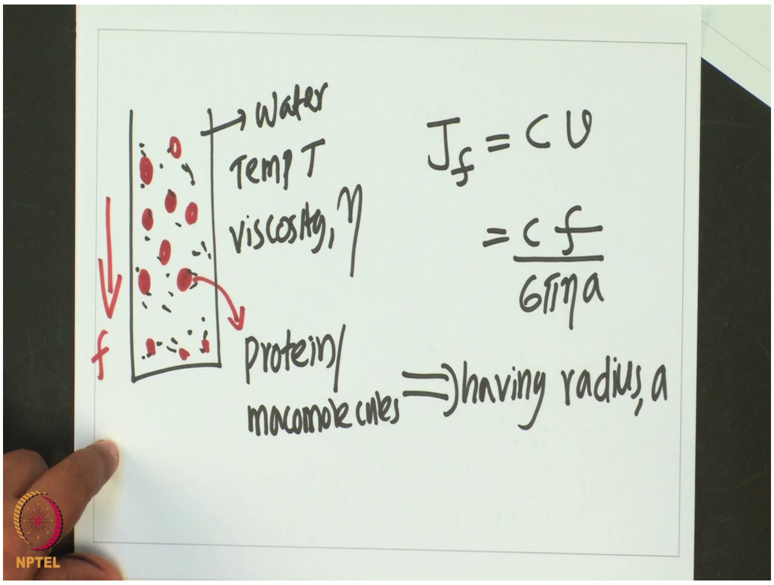

It is like a test tube in which of course, there is water everywhere. So, there is water 300 Kelvin. So, the water at room temperature or it is a some temperature T. So, this is water temperature T and of course, water has a viscosity eta is the viscosity. So, these are the property of the water and then; now you put lot of molecules in this which is much bigger than water and they will come down and they will come down because of gravity there will be the gravitational force will pull them down.

So, this is something that we all know that this will pull down and there is a flow of this protein molecules from top to bottom, it will say demand and this flow which we can estimate and the flow due to gravitational force which is J f which we know that is C times V where C is a concentration and V is the speed with which this would come and this V is related to the force and this can be written as C f by 6 pi eta a; where a is the radius of this particle. So, these are protein red is; so, this red things are protein molecules or proteins a slash other macromolecules it could protein or it could be anything macromolecules having radius a.

So, this are we assume that they are like a sphere therefore, we can say that they will flow down because of the force. So, the force here is the gravitational force and because of this gravitational force they will come down. So, that is something that we know because they come down they will sediment. So, there will be sedimentation and after some time if we look; they all will be down and a few of them will be below also. So, they will all come down and sediment at the bottom. So, if you look at after some time T what one would get one would get that one would get a picture which is I would not draw the water now would only draw the protein molecules.

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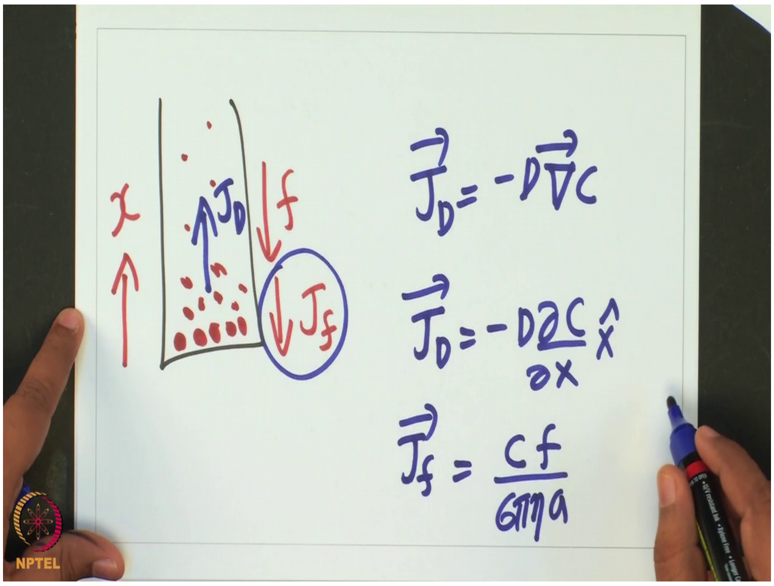

So, there will be like mostly at the bottom and few here and there. So, there will be mostly here at the bottom and a few here. So, I would call this as x direction. So, let us call this as the x direction and there is a force in this way and because of that there will be also a flow, in this way and they will all sediment down once this happens if you have a higher concentration here and a lower concentration here. So, when there is a higher concentration here and a lower concentration here there will be a diffusive flow in the opposite direction.

So, there will be a flow due to force f in this way, but there will be a diffusive flow J D in this direction. So, there will be a flow due to external force which is sedimentation in this way and there will be diffusive flow in the opposite direction from higher concentration lower concentration. So, what is the diffusive flow the diffusive flow we know which is k is written as J D which is minus D del C. So, let us do imagine this is a one dimension x. So, let us write this minus D del C by del x along x cap which is this way.

And so, this is the diffusional; diffusing current and the other one which the current downwards which we already know which is C f by 6 pi eta a. So, we know these 2 currents one current is due to one flow is due to the external field which will pull bring this protein down and once they are down they will go up and this would be the diffusive current from higher concentration to lower concentration and this is given by this now what is the C at equilibrium what is the concentration at equilibrium. So, it turns out that an analysis will show that higher concentration at when x is at here in lower concentration here and it can be argued which I would not discuss how it is coming.

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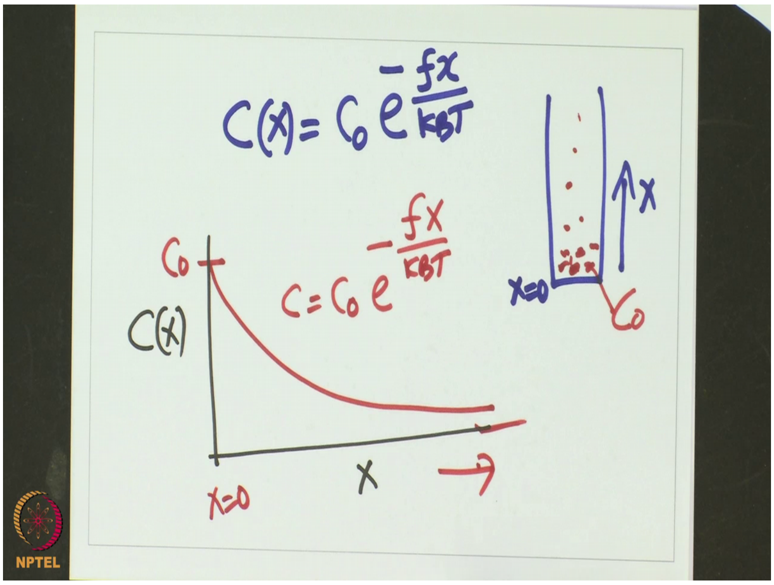

But from statistical thermodynamics and from other ideas one would one can show that C of x concentration as the function of x. So, that is concentration as you go along x would be some initial some concentration C 0 e power minus f x by KBT. So, fx is the energy force times distance and KBT is also energy. So, it can be shown that the concentration at any point. So, concentration at far away; so, this is x equal to 0. So, there will be very high concentration here. So, an x equal to 0; here the concentration is C 0.

So, at x equal to 0 that is at the bottom there will be high concentration. So, which will be C 0 and as you go the concentration will decrease. So, the if I plot C of x versus x it would be an exponentially decreasing concentration like this where this is C 0 and this relation is C is equal to C 0 e power minus fx divided by KBT where f is the force and x is the distance and this would be the profile of concentration; that means, high concentration at the bottom x equal to 0 and very low concentration as you go along x upward.

So, this is this can be shown from statistical thermodynamic arguments that the concentration profile will have this. So, known this Einstein knew this and known this. So, we know 3 facts one we know that there will be a flow.

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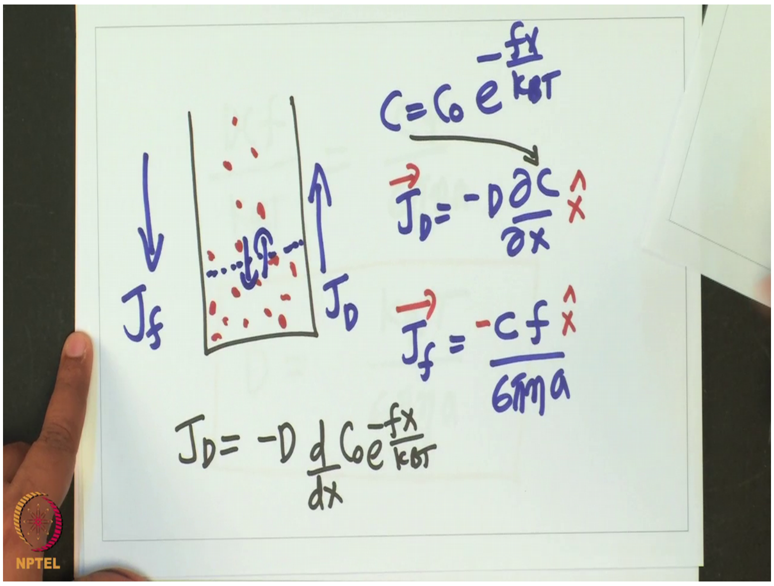

So, what is; so, let us consider 3 facts that we know what we know that there will be a concentration gradient and there will be a concentration low very high concentration at the bottom has smaller small concentration top and there will be a flow down due to the force the molecules will be pull down by gravitational force and there will be a flow in this way because of the diffusion and the concentration is C 0 e power minus fx by KBT and we know that J D is minus D del C by del x. This is the magnitude and this will have the magnitude for this would be C f by 6 pi eta a.

So, we know this. So, now, what one has to do is that at equilibrium when the system is in equilibrium this flow will balance with this flow. So, that is if this is equal and opposite this the directions are opposite and if their magnitudes are equal. So, whenever their magnitudes are equal and the directions are opposite. So, f will have a direction which is minus x cap. So, this is f if I put a vector sign. So, let us put a vector sign carefully. So, this would be x cap here and this would be below towards the minus x. So, I would write x cap with a minus sign. So, this would be coming down towards minus x f is a magnitude of the force and x cap is the direction minus x cap is the direction of this diffusive flow.

So, if they are whenever they are whenever their magnitudes are equal. So, that is this magnitude is equal to this magnitude they will be when this flow will balance. So, when this flows balanced with each other what will we get. So, let us equate these 2 flows. So, if you substitute this C here we can show the J D will be equal to minus D del C by del x. So, C is this. So, if let us the derivative of this would give us. So, if the del; if I calculate del C by. So, by substituting this C here and if I calculate the derivative of this what I would get I would get that D by dx of C 0 e power minus f x divided by KBT this; what I would get.

So, let us recalculate these 2 things. So, let us first recalculate JD.

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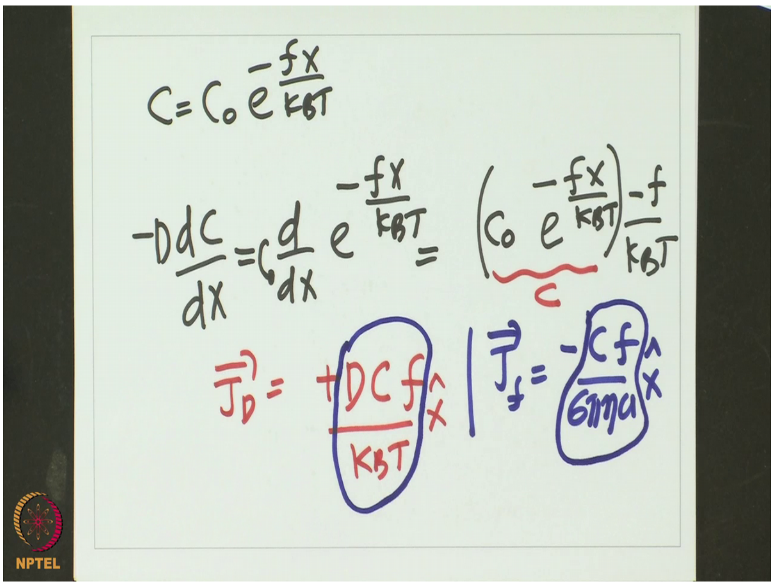

So, what we know we know the C is C 0 e power minus fx by KBT that is what we know and minus D dc by dx would be D by dx of e power minus fx by KBT and there is C 0 here this would give C 0 derivative of this would give you e power minus fx by KBT and a factor which is minus fx by KBT will come. So, times minus f by KBT. So, this would be this and the; if I substitute the full J D would be minus D times this thing is my C itself. So, C minus f; so, this would become plus f by KBT and there will be an x cap here.

So, this will be the diffusive current. So, J D if I substitute if I substitute J D is equal to minus D del C by del x since I took a ordinary derivative here because only function of x I would get minus D C this would be C dc by dx with the minus f by KBT minus and this minus will cancel and become a plus f plus sign here. So, DC f by KBT along x cap will be the current and the other flow which you already know is that J f is minus C f by 6 pi eta a x cap.

So, if they are the total the; if they are equal and opposite. So, one has to equate these 2 and they have to be equal and then they have to be opposite. So, if I equate this and consider an equal and opposite I can equate these 2 and with a fact that they are opposite. So, I can essentially equate the magnitude of this. So, if I equate the magnitude of these 2 things. So, that is let us equate the magnitude of this which is DCf by KBT and the magnitude of this which is C f by 6 pi eta a. So, if these 2 are equal these currents will be equal in magnitude and opposite in direction.

So, this is along the plus x direction and this is along plus x direction this is along minus x direction. So, if I if these magnitudes are equal whatever I have put in this circle in this; this is a magnitude; if they are in equal magnitude will be equal the direction will be opposite. So, the flow that is be equal in magnitude, but opposite in direction at that when they are equal in magnitude and opposite in direction both the flows will cancel and on an average the number of proteins at any point would remain a constant.

So, let us equate these 2 this equal to this. So, what do I get? I would if I equate these 2 things.

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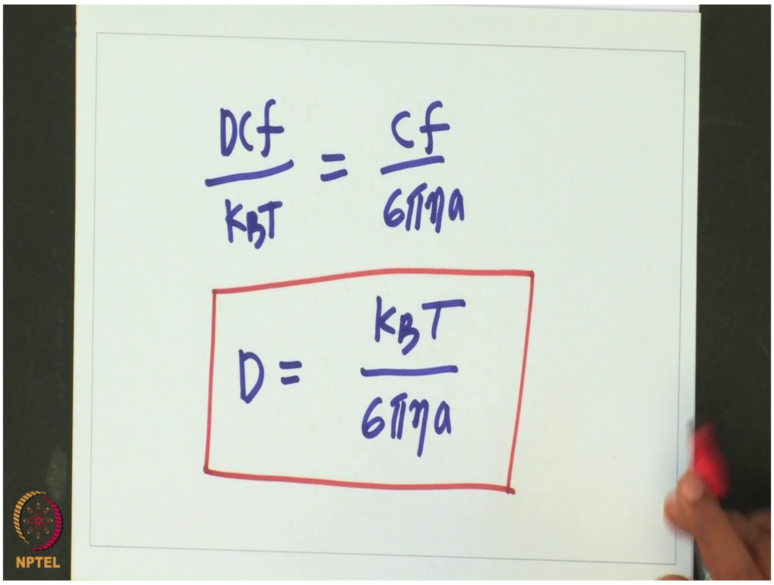

I would get DC f by KBT is equal to C f by 6 pi eta a. So, this would C and C f would cancel and this would tell me D is equal to KBT divided by 6 pi eta a; this is the famous Einstein relation. So, Einstein showed that D which is the diffusion constant is equal to KB where KB is the Boltzmann constant T is the temperature eta is the viscosity a is the radius of the protein assuming that it has a spherical shape.

So, the folders globular proteins one can approximate to sphere which has a radius of size a. So, one can show from simple calculus that by equating the current which is flowing the diffusive current up and the flow due to force down if I equate these 2 which are this and this if I equate these 2 assuming this C is equal to C 0 e power minus f x by KBT, I would get this that these are the 2 currents J f and J D and their magnitudes are shown here in this circle in this a in this here I have circled it. And if I take these 2 quantities and equate them their magnitudes will be the same if their magnitudes are equal; they will have a opposite direction what does that mean; that means, at any point x there will be a flow down which is equal to flow up; that means, on an average at any point x the J here is equal this way and equal this way if they are equal. They are on an average the number of particles will remain a constant at any point in x and that is the equilibrium.

And at equilibrium one would say that at equilibrium you would get a relation and that relation is the famous Einstein relation which says that D is equal to KBT 6 pi eta a. So, this is the important relation for now let us understand this D is proportional to temperature higher the temperature more the diffusion constant lower the viscosity higher the diffusion constant higher the viscosity smaller the diffusion constant and a the bigger the particle smaller the diffusion constant.

So, this diffusion constant depends on primarily 3 qualities temperature viscosity and the size of the particle now let us calculate this KBT for typical biological molecule which is of our interest. So, let us take a pattic some protein like let us say a actein or any protein of our interest which has size of the order of few nanometers. So, let us take a approximately 1 or 2 nanometers. So, if I assume diameter of 2 nanometer; it will have a radius of one nanometer.

So, let us take let us assume if you have a small protein which has a radius of one nanometer at 300 Kelvin what would be our 3 10 Kelvin let us take 300 Kelvin for convenience this is room temperature approximately close to room temperature what would be the diffusion constant.

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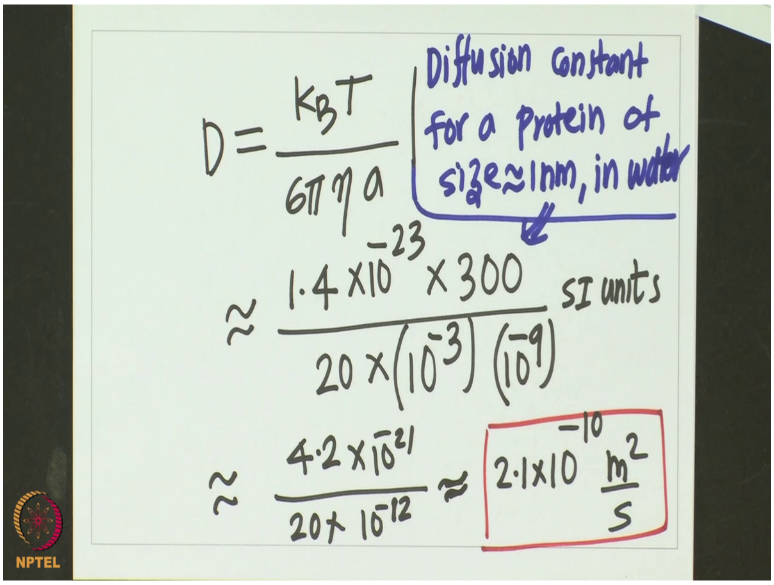

So, let us calculate that number here. So, the number D we would calculate D is equal to KB T by 6 pi eta a. So, if you assume water viscosity of water we have to substitute boltzmann constant we have to substitute temperature we have to substitute.

So, approximately the Boltzmann constant has the approximately this has 1.4; 1.4 times 10 power minus 23 in si units that is what approximate number and temperature is 300 Kelvin and 6 pi is let us take approximately 20 which is around 18 point something. But let us take 20 as order of magnitude if we calculate eta which is viscosity of water and it is going to be 10 power minus 3 in si units as viscosity of water in si units is 10 power minus 3 and a is of the order of nanometer.

So, in si units nanometer is 10 power minus 9 meter. So, everything is in si units. So, if I substitute everything in si units I should get the si unit of diffusion called D is meter square per second. So, I should get the answer finally, in meter square per second. So, let us do this for. So, this is diffusion constant what are we calculating; we are going to calculate diffusion constant for a protein of size that is radius one nanometer in water in water that is what we are calculating here.

So, diffusion constant for a protein of size one nanometer in water; so, if I substitute here what I would get is that 3 into 4; 1.4 is like four point 2 into 10 power minus 21 divided by 20 times. This is 12; 10 power minus 12. So, this is 9 and there is a 20 here in this. So, this is approximately 2. So, this would be 10 power minus I multiply the 10 power minus 11. So, this would be 10 power minus 10 2 2. So, this will be 2.1. So, 2.1 into 10 power minus 10 meter square per second.

So, this would be a approximate number I urge you to calculate it this is approximately as you recalculate this. So, this would be the typical diffusion constant for a protein having a particular size of the order of one nanometer. So, 10 2 into 2 a roughly 2 into 10 power minus 10 meter square per second would be the approximate diffusion constant for a particle having size one nanometer. So, this is we now know how to calculate diffusion constant for any protein the only thing we have to know is rough globular size of the protein the radius of the protein globule.

If I know that at room temperature in water or whatever viscosity you take if we take the viscosity in a cytoplasm you take slightly higher viscosity roughly 5 times higher, then you would get a slightly different number which is 5 divided by 5. So, it will be like 5 times less than that that is only difference, but approximately roughly of this order. So, we could now calculate the diffusion constant. So, to summarize what we learnt we learnt that one can very easily derive Einstein's relation by doing just doing the following.

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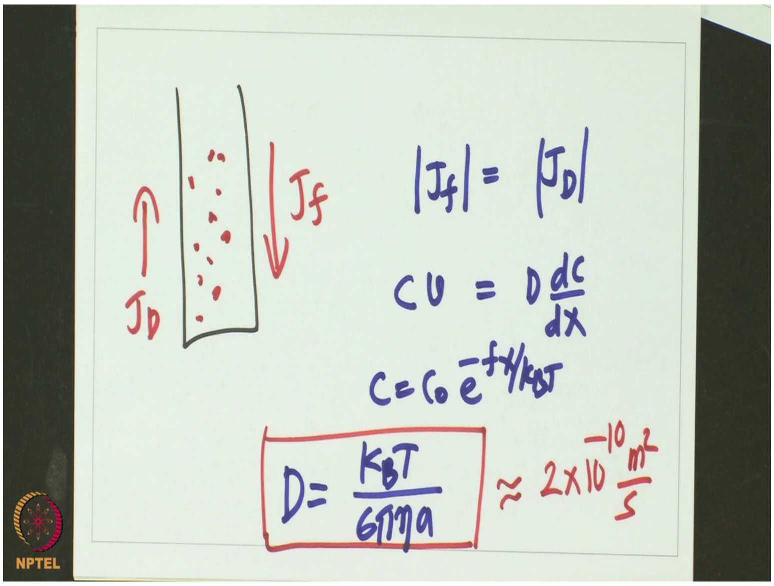

By considering protein molecules in water they will come down due to the external force there will be a flow they will go up due to diffusion and when these 2 currents are equal and opposite when this currents their magnitudes J f is equal to JD, but they have an opposite direction.

So, if then their magnitudes are equal then the directions that you know already the directions are opposite. So, when they have equal in magnitude by equating these 2 things we can get that that is if you equate cv is equal to D dc by dx where C is equal to C 0 e power minus fx by KBT by equating. This we got this relation dc equal to KBT by 6 pi eta a and we computed this; this is the famous Einstein relation this relates diffusion equation to temperature and viscosity and this we calculated which was approximately 2 into 10 power minus 10 meter square per second for a protein of one nanometer.

So, this is the summary of this lecture with this will stop and continue in the next lecture. Bye.