Transport Phenomena.
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Lecture-46.
Mass transfer (Continued).

So today we are going to solve, this is going to be a tutorial and we would be looking at a specific problem and would try to use the shell mass balance, more correctly the shell species balance to evaluate certain quantities and as an example we have taken the dissolution of a drug inside our intestine. So as you are aware of many of these drugs are time released drugs, that means it is going to dissolve slowly in the juices present at in our intestine and it is going to be active over a prolonged period of time. So this kind of time release drug, the way they are manufactured is that the drug is going to be coated with a specific coating through which the drug molecules will slowly diffuse and get dissolved in our, in the intestinal juices.

So far as long as we have this diffusion, so it is not going to be a rapid diffusion, it is not going to dissolve instantaneously, it is going to dissolve and be active over a prolonged period of time. So we are going to start with a specific drug which is probably made in a pellet of cylindrical sizes of certain radius and length and it is going to be coated with an inner coating, so it does not serve any purpose other than it reduces the dissolution of the drug. So the drug has to diffuse through this coating, reach the other end where the convective conditions will result in a specific convective heat, convective mass transfer coefficient.

So the drug molecules that diffuses through the inert layer comes on the outside of the inert layer and will be will be carried away from the drug, the drug, cylindrical shaped drug and will be absorbed at our intestine. So this is the problem which we are going to model and we are going to solve for it.

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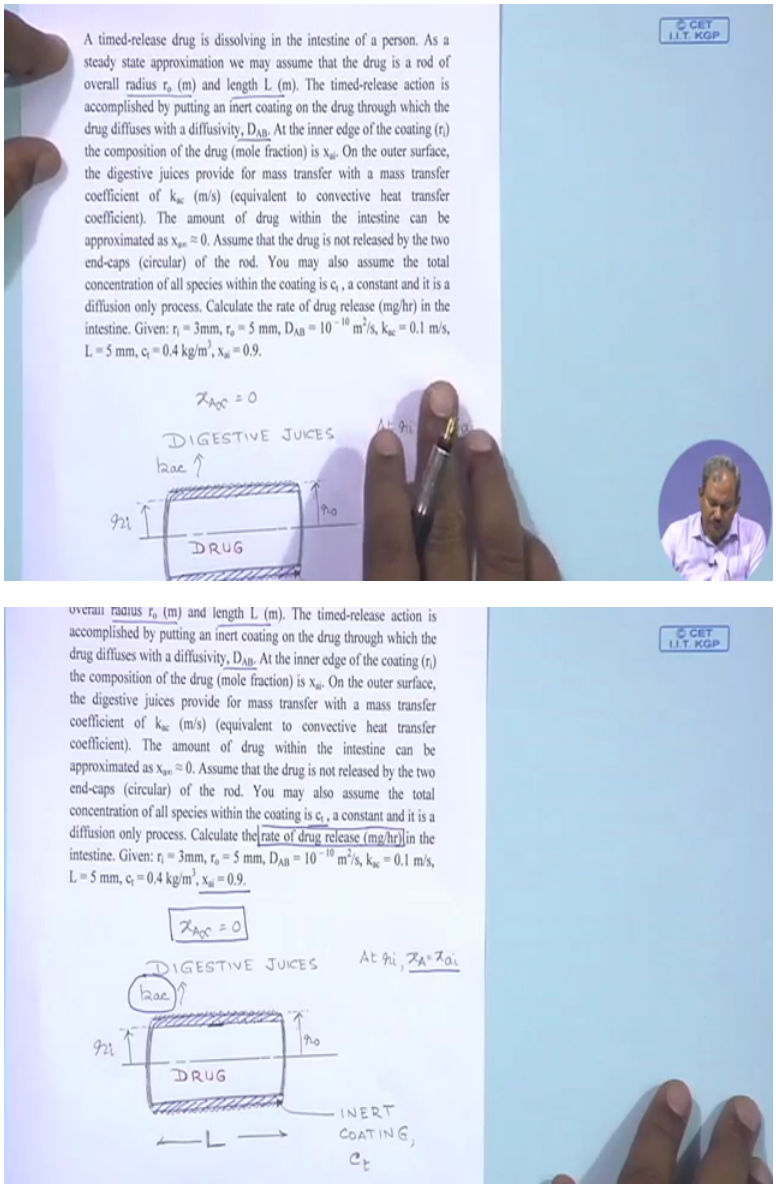

So the specific problem that we are going to look at is as I mentioned before a time release drug is slowly dissolving in the intestine of a person and we are going to use the steady-state approximation and we will assume that the drug is a rod of overall radius r0 and it has a length equal to L and the time released action as I mentioned before is accomplished by putting an inert coating on the drug through which the drug diffuses with the diffusivity which has been denoted by DAB. At the inner edge of the coating, let us look at the figure which I have drawn for this, at the inner edge of the coating, so this is the drug, the white portion that you see here is the drug, it is cylindrical in shape with 2 endcaps.

And at this point, that is at the inside of these inside of the inert coating, at the inside of the coatings, that means at r equal to r i, where r i is the radius of the cylindrical drug pellet, the

concentration of the drug is maintained, the mole fraction is maintained at X A equals XAI. And the digestive juices which are present on the outside of the drug that we have, it maintains a coefficient of mass transfer which is similar to that of a convective heat transfer coefficient as denoted by the KAC.

So any molecule which comes on the outside through diffusion, through this inert layer which is the shaded, the blue shaded region, the drug molecules will then be moved away by a convective mass transfer coefficient and the concentration at the outside of the outside of the drug at a point far from it is maintained at 0 concentration. So XA infinity is equal to 0, the drug, it has also been assumed that the drug is not going to be released by these 2 endcaps. So the drug is only going to be released through the inert core, that is through the cylindrical surface of the drug. So as I said on the outer surface, the digestive juices provide for a mass transfer coefficient which is denoted by KAC, units of metre per second and the amount of drug within the intestine can be approximated as XA infinity to be equal to 0.

So at a point far from the far from the drug, the concentration is assumed to be 0 and there is also not released by these 2 endcaps. And you can also assume that the total concentration of all these species within the coating is CT, which is a constant, so there can be other species present in this coating apart from that of the drug and the total concentration of everything which is present inside the coating material is denoted by C suffix T which we can assumed to be a constant. And we will assume that it is a diffusion only process and we need to calculate the rate of drug release in milligram per hour in the intestine.

So how much of drug is going to diffuse through the inert layer, come to the other side and get convected out of the drug into our intestinal juices. So this is we have to need to calculate the rate of drug release in milligram per hour and the geometric and other information which are provided is the inner radius of the drug that is without the coating is r I which is 3 millimetre and when you put the inert coating on it, the radius is going to be equal to r0 which is 5 millimetre, the diffusion coefficient is 10 to the power - 10 metre square per second, the convective mass transfer coefficient is provided as 0.1 metre per second, the entire length of the drug is 5 millimetre, the concentration including the drug, concentration of all the species present in the inert material, inert cover including that of the drug a 0.4 KG per metre cube and XA I which is the mole fraction of the drug at the inner layer of the coating, that means at this point is equal to the mole fraction is equal to 0.9.

So what we need to find out is the rate of drug released in milligram per hour in the intestine. So you can see this is just a diffusion only process and if you take a thin slice in the inert core, inert cover of the drug, then we should be able to write what is the shell species balance, the species in this case is that of the drug. So the drug diffuses through the inner core, reaches the outside and will be will move out of the of the drug into the intestine. So it is a diffusion only, one-dimensional diffusion only process where the drug is moving only in the r direction.

So in, so therefore we understand that the concentration or the mole fraction of the drug is going to be a function of r, do not going to be function of length, that is Z in here and definitely it is not going to be function of Theta. So irrespective of the position of the shell with respect to Theta, the concentration, the mole fraction is going to be same at all Theta. So we are going to assume a shell which lies inside the inner core and we are going to make a balance and no reaction is taking place. So we are going to make a balance of the drug molecules coming at the core at, coming at the shell, going out on the other side through, through the on the other side of the shell.

And in the shell there is no reaction which is taking place. So the flux multiplied by the area and the area is simply going to be equal to twice pie r times L, this is the inner surface area of the imaginary shell. So twice pie r times L, that is going to be the area through which the diffusion takes place. So that multiplied with the radial molar flux of the drug, that is going to be the amount of drug, moles of drug which is coming to the inner surface per-unit time.

On the other side the radius is going to be of the imaginary shell, the radius is going to be r + Delta r and will have another flux which goes out of it. There is no generation term, no depletion term, that is no reaction is taking place and at steady-state rate of a molecules in, rate of in - rate of out less 0, since there is no generation and since it is at steady-state, the right-hand side of the species conservation equation will also be 0. So essentially what we are saying is that the rate in - rate out is going to be equal to 0. So that is the species balance equation, the species in this case being that of the drug, so we will start from that point.

Therefore, I hope the figure is self-explanatory. So the drug, the coating, the outside where we have the digestive juices, the convective coefficient and the boundary conditions provided at the inner core, the mole fraction is provided and at a point far from the far from the drugs the concentration of the drug in the digestive juices would be equal to 0. rI, r 0, the values are provided, the length is provided, the total concentration of all the species present in the inner

core is provided and the mole fraction of the drug at the inner core, at the inner core is also given. So we will start with the derivation of the governing equation.

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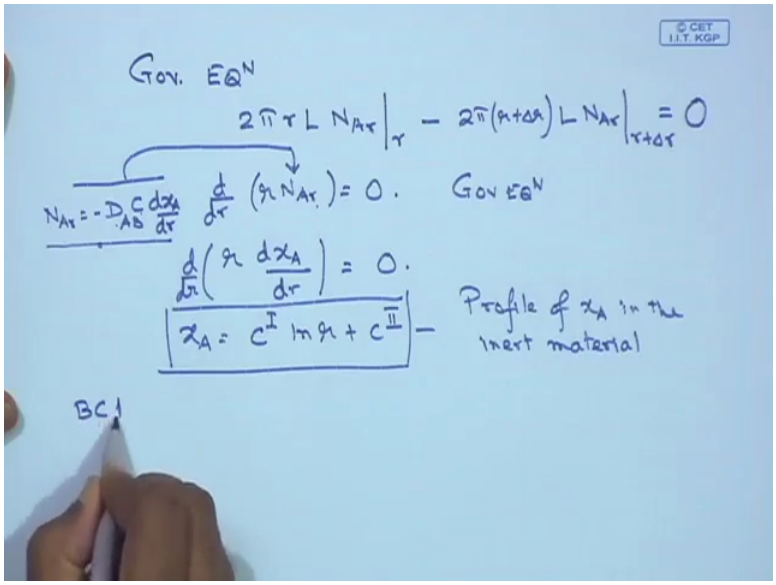

So my governing equation in this case as I have mentioned in which is twice pie r times L, so that is the area multiplied by the flux evaluated at r, at any r would be equal to twice pie r + Delta r times L, that is the outside area of the imaginary shell multiplied by NAr, everything evaluated at r + Delta r, since there is no reaction and since we are talking about 0, at steady-state, this is going to be equal to 0. So what you get by dividing both sides by r, what you get and taking the, using the definition of the 1st derivative, we would simply get this to be equal to 0.

So this is your governing equation and which can then be integrated in order to obtain r times and after you, since it is a diffusion only process you can simply write N Ar to be equals - DAB times C which is the concentration times D XA by Dr forces are you plug this in here and what you would get out of this is that since C is a constant, Dab is a constant, they will get, we can cancel this and what we have then is r times D XA Dr and D Dr of that, at steady-state would be equal to 0. So we have used Fick's law for a diffusion only case plug that in for the molar flux of the component A in the r direction and the governing equation and since C and DAB are constants, this is going to be my governing equation.

So once you integrate it twice, you are simply going to get XA to be equals C1, where C1 is one constant of integration times ln r + C2. So this would be the profile, profile of XA in the inert material. Had this been a case of constant surface area, for example in a plain wall, the

distribution is going to be linear. But in this case as the drug molecules move upwards, it experiences more larger. So for these types of cases, for cylindrical cases, the concentration distribution, exactly like temperature distribution is going to be a logarithmic function of the radial position. So therefore the mole fraction of A which is the drug inside the inert material in absence of any reaction will simply follow a logarithmic distribution.

And that is what we have obtained in here and we now need to solve for C1 and C2, the 2 constants of integration using the boundary conditions which are available to us. One boundary condition is straightforward, that is known concentration at a specific location. We understand that at the inner core of the inert material, the mole fraction of A, the drug molecule is specified.

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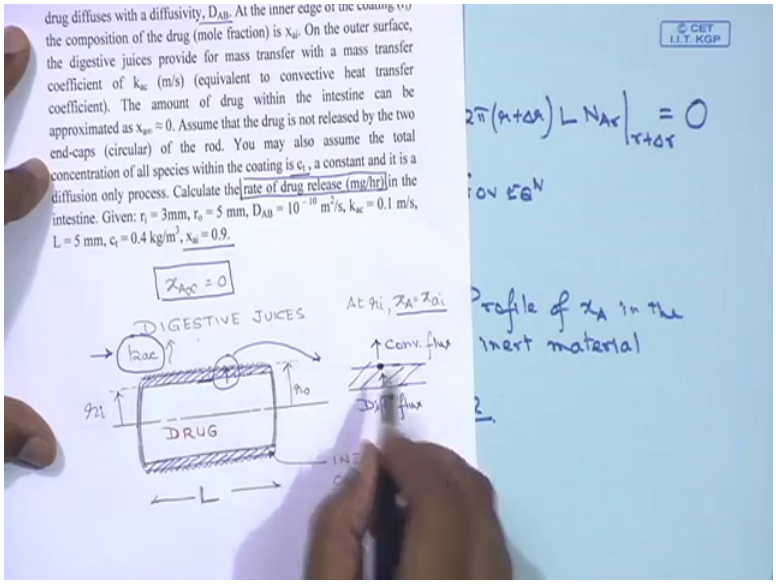

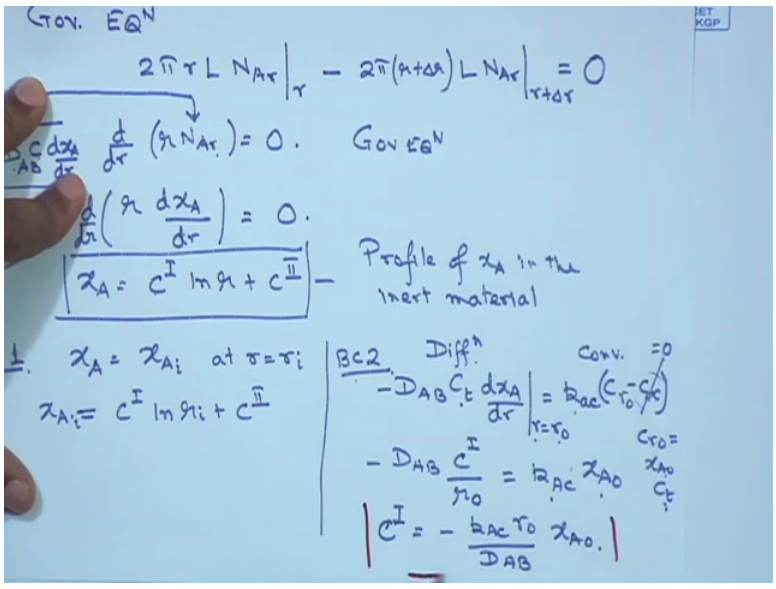

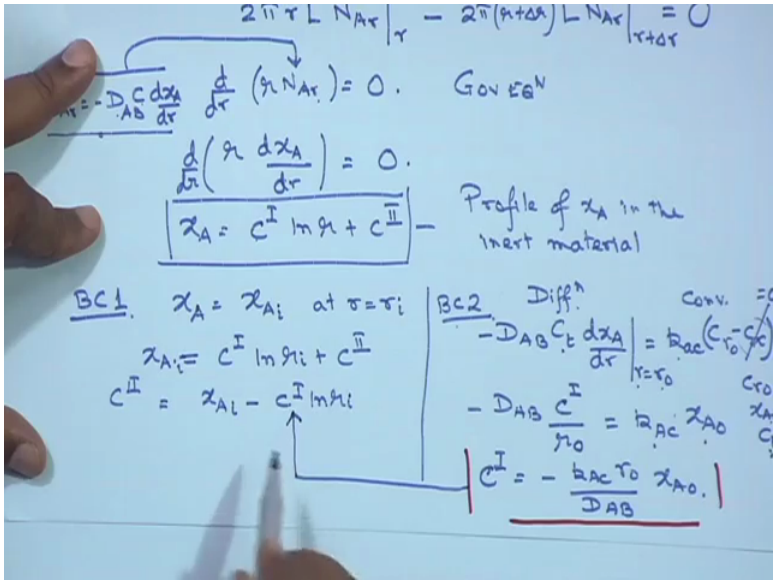

So the 1st boundary condition, the boundary condition one would simply be equals that at XA, the mole fraction is going to be equal to X AI and it r equals rI. So this is going to be the 1st boundary condition, so when you put the 1st boundary condition in here, it is simply going to the X AI is equal to C1 times LN r I + C2, so this is going to be my relation one. And the 2nd boundary condition, the boundary condition 2 will be on the outer surface on this surface, on the outer surface of the coating. So at the outer surface of the coating the diffusive flux, the diffusive flux of the drug molecules which are reaching, so if I take this as my, as an enlarged view of this region, what you would get is the diffusive flux which is reaching at this point must be equal to the convective flux.

So diffusive flux must be equal to the convective flux. So the amount of A which reaches by diffusion to the outer layer of the coating must be convected out due to the convective condition maintained by the digestive juices with a convective mass transfer coefficient denoted by KAC. So if we write the equivalent of Newton's law to denote the convection of species and the Fick's law for the diffusion by which the drugs reach at this point, the convective diffusive boundary condition together would give us - Dab times total concentration D XA DR evaluated at r equals r0 is equal to K AC, that is the convective coefficient times concentration at r0 - concentration at infinite distance, concentration at infinite distance.

So this is essentially the diffusion and this is convection, so all the control surface which characterises the outer surface of the coating, diffusion of A must be equal to the convection of, convection of A away from the digestive from the drug from the drug into the intestinal juices. So what we can write this as - Dab and D XA Dr, if you look at D XA Dr from here,

you simply going to get this to be equal to D XA Dr is going to be C1 divided by, it is evaluated at r0, so this is going to be C1 by r 0. If you integrate it, if you differentiate it once, D XA Dr would be C1 by r and since I am evaluating at r equals r0, it is simply going to be C1 by r0.

So this is going to be the left-hand side, and on the right-hand side it is going to be K AC times X A 0. We understand that Cr0 is XA, Cr0 is equal to XA 0 times CT. So C, and CX a infinity is 0, so this part is going to be equal to 0 and what I have left with after I cancelled it is the tea from both sides, what I am left with K AC times XA 0. So this is one condition which is obtained by quitting diffusion and convection and identifying that C0 which is X, with C infinity, which is X A infinity multiplied by CT and we know that C infinity, XA infinity is 0, so therefore this part is going to be 0, no drug, you have very small concentration of drug in the intestinal juices, so this can be equated to 0 and we cancel CT from both sides.

So therefore you can get the expression of C1 as equals - K AC times R 0 divided by Dab times X A0. So the expression for the 1st integration constant can be obtained by, through the use of the 2nd boundary condition. So this is what we have obtained as the expression for the 1st integration constant. This can now be put in here, so therefore you would get C2 which is the other boundary condition would simply be equals X AI - C1 ln rI, just this one. And then I am going to put the expression for C1 in here to obtain what is the expression for C2 going to be.

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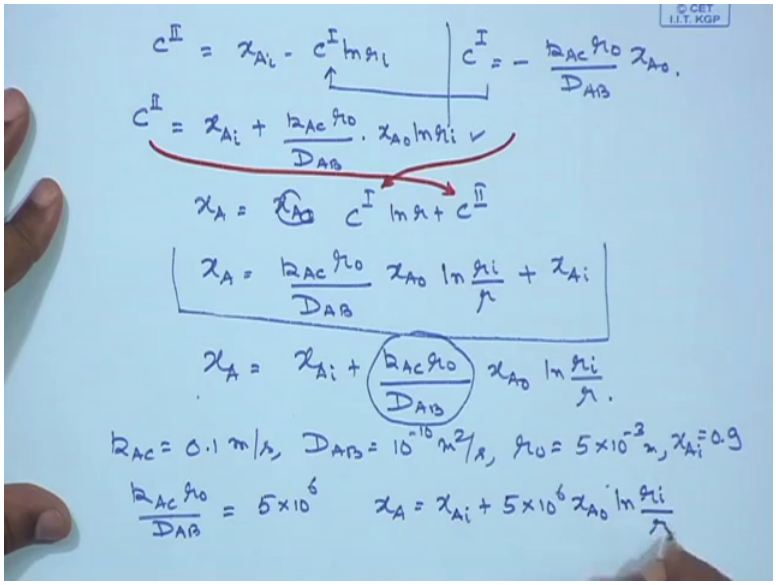

So I write C 2 once again in here as X AI - C1 ln r I and I have already obtained C1 to be equals - K AC r0 by Dab times XA0. So I think it is straightforward but if you have any questions, please email to me and if there are any questions, I will clarify, I will try to clarify that I will try to clarify that. So with this I come to the expression of C2 and once I put this in here, what I am going to get is C 2 is equal to X AI + because of this -, it is going to be K AC r0 by Dab times X in 0 ln rI. So now I have an expression for C2 as well. So if I go back to my original expression of XA to be equal to X A, XA to be equals C1 ln r + C2 and plug-in the values of C1 and C2 in here and do a little bit of simplification, what you are going to get is XA equal to K AC r0 by Dab times X A 0 which is the expression for C1 times ln rI by r + X AI.

So this is the expression, total, overall expression for XA that you are going to get out of this relation. So this is the, this is the final expression X A2 be equals X, written in the same way, in a more general way times r0 by Dab times XA0 ln rI by r. So what I need to do next is, we need to plug-in the values inherent and the value that are provided in the problem, X AI as 0.1 metre per second, Dab is provided as 10 to the power - 10 metre square per second, R 0 is 5 into 10 to the power - 3 metres, X AI is equals 0.9. So when you when you put this, this one is K AC r0 by Dab, when you plug-in the numbers, they will be equal to 5 into 10 to the power 6 which would give you X say to be equals X AI + 5 into 10 to the power 6 XA0 from this relation ln rI by r.

So now I have the 1st part of the problem which asks what is the, 1st part of the problem that we need to calculate the rate of drug release. So the 1st thing that I should do is find out what is the concentration distribution, so I have got an expression for concentration distribution in here.

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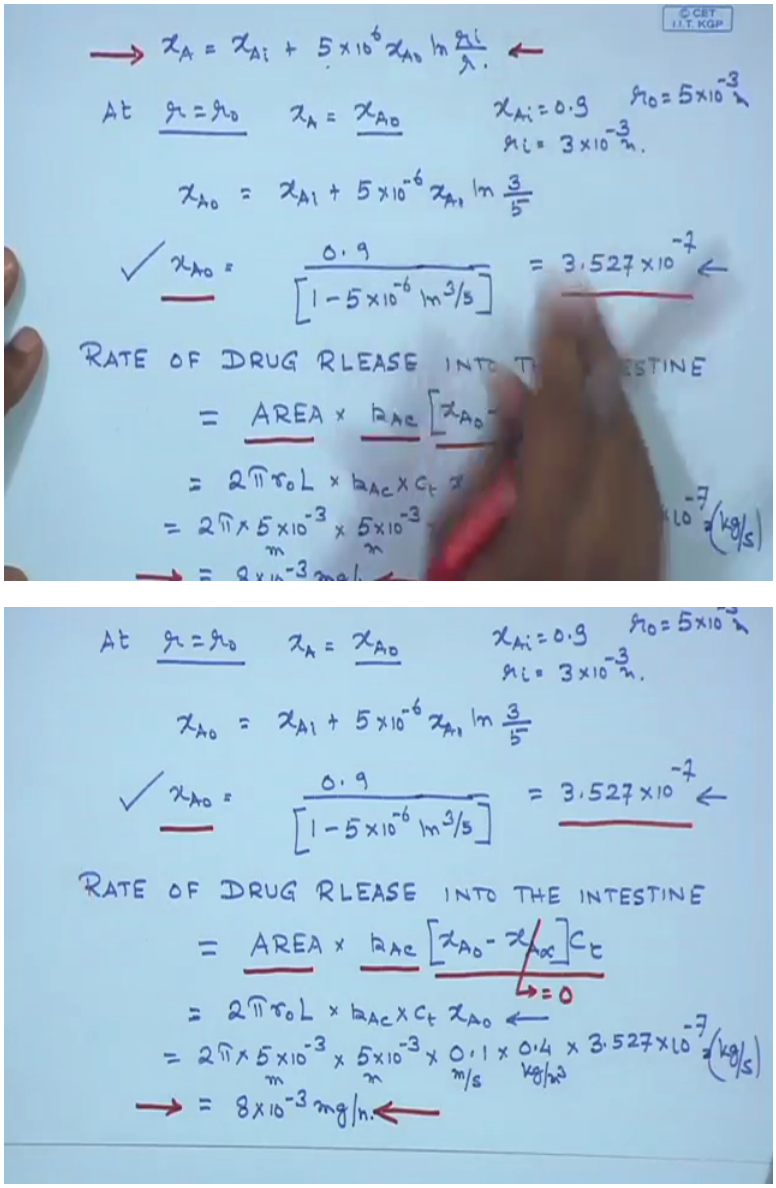

I will start this, I will write it once again that XA is equal to XAI + 5 into 10 to the power 6 XA0 ln r I by r. Okay. So we realise that at r equals r0, that means at the outer edge of the inert coating, my XA would simply be equal to XA0, let us call it at XA0 and we understand that at XAI is equal to 0.9, the value of rI is equal to 3 into 10 to the power - 3 metres and r0 is equal to 5 into 10 to the power - 3 metres. So when you when you put these values in here, so what you are going to get is XA0, which is the concentration, sorry, the mole fraction of component A at the outside of the inert layer is simply going to be equal to XA I +5 into 10 to the power - XA0 and ln instead of rI it is going to be 3 and r0 is simply going to be equal to 5.

So XA 0 would be equal to 0.9 divided by - 5 into 10 to the power - 6, when you bring this XA0 to this side, 5 into 10 to the power – 6 ln 3 by 5 and this would turn out to be 3.527 into 10 to the power - 7. So it essentially tells the concentration of the drug on the outside is simply going to be 3.5 into 10 to the power -7. The next, the next that is remaining is rate of drug release which has been asked, rate of drug released into the intestine that as a drug designer you must find out and we understand that since I know XA0, I should be able to equate the, multiply the convective movement of the drug away from the inert core, away from the outside of the inner core to the digestive juices.

So I am going to have this as KAC multiplied by XA0 - XA infinity times whatever be the total concentration in here. So ideally if you look at, the concentration, the convection, total amount of convection of the species away from the outer core of the inert material is simply going to be the convective mass transfer coefficient multiplied by the concentration difference. So that when you multiply with the area, outer area of the inert coating would give you in KG per second, in SI units, in KG per second, what is the total amount of drugs that will diffuse through the inert layer, reach the outside of the net layer and by a convection process initiated by the movement of the intestinal juices inside the intestine that is going to get dissolved.

So it is going to give you the dissolution rate of the drug in our intestine. So if you see this is the area, this is the convective transfer coefficient and this is the concentration difference. So this is area, this is convective mass transfer coefficient and this is nothing but the concentration difference in here. We understand that this is XA infinity is assumed to be 0, that means no drug exists in the intestinal juices. So if I substitute, if I put the expression for area, it is simply going to be twice pie r0 times L, it is a cylindrical area and only the side area is going to contribute, the endcaps are not going to be, endcaps, they do not contribute to the movement of the drug, so the area over here is simply going to be outer area is going to be twice pie r0 times L times K AC times CT times XA0.

So this is the total amount of drug which gets dissolved in the intestine and when you put the values in here, twice pie times r0 is 5 into 10 to the power - 3 in metres. L is again 5 into 10 to the power - 3 in metres, the value of K AC is provided as 0.1, this is in metre per second, then CT is given, the total concentration of all the species present is given as CT as 0.4 KG per metre cube into the value of XA0 which we have obtained from here. So into 3.5 to 7 into 10 to the power - 7, this being a mole fraction, obviously it does not have any units. So if you

look at the units over here, the overall, that will unit is simply going to be equal to in KG per second.

So the whole, the rate of drug release we have a painting in SI units which is in KG per second. When you evaluate this, this is going to come to be equals 8 into 10 to the power - 3 milligram per hour. So that is the dissolution rate, that is the dissolution rate of the drug in the intestine. So you see that this is a pretty simple problems which is, when you start with a balance in an imaginary shell across which one component is diffusing, it is a diffusion only case, so you do not have to consider convection. So the Fick's law, the simplified form of Fick's law only for diffusion is to be used in this case.

So you get D DZ of N AZ to be equal to 0 and it is a radial, DZ of r N AZ, D Dr of rN AZ to be equal to 0. Since it is a cylindrical system in which as the as the molecule, as the drug molecules diffuse out, it encounters a bigger area, larger area. So therefore the distribution of the concentration or the mole fraction of this drug inside the inert material is going to be a logarithmic function of the radial position.

There are 2 boundary conditions which are needed, we identified the boundary conditions to be known concentration at a given location which is at r equals r I and at the outer edge of the net layer we have equated taking that to be my control surface we have equated, we have equated the diffusive flow of drug up to that point through the solid inner core must be equal to the convective flow, convective flow out of the drug molecule from the outside of the inert core.

So equating the diffusion and the convection we could evaluate what is the 2^{nd} boundary condition and putting the 2^{nd} boundary condition into the expression of XA which is the mole fraction of A, we could also obtain what is the 1^{st} boundary, 1^{st} constant of integration. So we have obtained this as my, this as the concentration profile after plugging in the, plugging the numbers in, we have obtained what is the concentration distribution and since we know at r equal to r0, let XA is equal to X is 0, we obtained what is the numerical value of X is 0 after putting in the values that we know and the rate of drug release is simply the product of area, the convection coefficient and the concentration distribution.

See the concentration distribution here which is the common practice in many mass transfer mass transfer cases is expressed not in terms of concentration difference but in terms of the mole fraction difference and the mole fraction multiplied by the total concentration would

give you the mass, would give you the mole fraction of component A at 2 locations. We know at infinity, at a point far from the drug, the mole fraction is 0, so we need, we put that equal to 0 and we get a compact expression and obtain what is the dissolution rate of the drug in our intestine.

So next I would also upload a few other problems on mass transfer that you can try on your own. And if there are questions I would I would provide you with the answers as well with short pointers of how to solve them and this you have any questions then we can discuss it further off-line. In the next class what I am going to do is, the same way I have developed the equation of energy and equation of conservation of momentum, the same way I would do it for a species balance equation which would be straightforward since we are only going to deal not with momentum transfer, heat transfer, we are simply going to write the conservation equation of a species.

It could react with another species, it could be, it could be a process which is transient in nature, so I am going to write, I am going to derive the general form of the concentration distribution of one species as a function of XYZ, the positional coordinates as well as time. And when I have that in cylindrical coordinates, Cartesian coordinates and spherical coordinates, then you as before no longer would need to do the shell momentum, shell mass balance anymore. You simply pick the equation that in the right coordinate systems and starts with the species transport equation with the at the appropriate coordinate system, let us say cylindrical coordinate systems.

Cancel the terms using simple logic and what you would get at the end of the process is your governing equation for the species transport in that case. It is going to be extremely important for to deal with cases where the geometry is complicated, where you may have the concentration varying in X and Y directions or more importantly when we are dealing with transient mass transfer situations. So that would be the topic of the next class.