Course: Adsorption Science and Technology: Fundamentals and Applications

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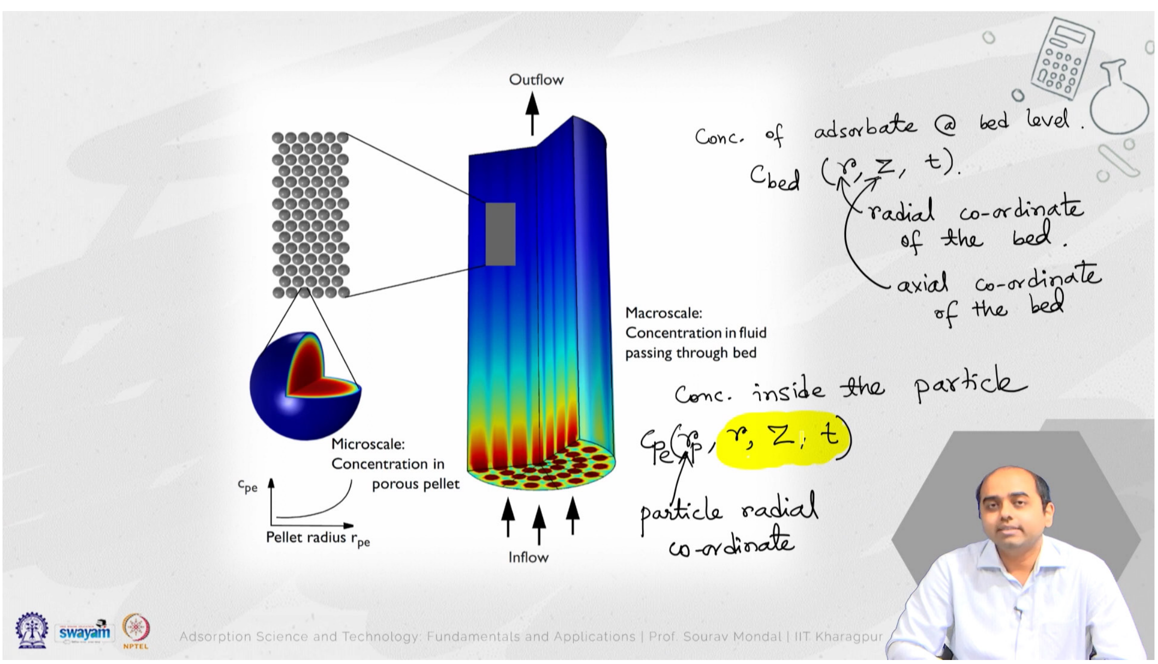
Week 06

Lecture 26 | Fixed Bed Design: Multi-Scale Model

Hello everyone. Welcome to this new week of this course on adsorption science and technology. So, in this week we are we will be continuing from the previous week related to fixed bed adsorption and we will see couple of scenarios where this fixed bed adsorption is put into practical use towards the you know after a few lectures in this week. So, today I am going to talk about the role of multiscale you know model in fixed bed design. So, for the models that we have been talking about whether you talk about this constant pattern behaviour analysis, this Thomas model, then we talked about this you know this Adams-Bohart model or this whatever the other modules that we have talked about Clark model, Yoon-Nelson model. All of these models is essentially or are essentially considers the dynamics in the bed, but it fails to connect with the intra particle or inter particle you know phenomena. And this is particularly very relevant or essential when the intra particle physics becomes quite dominating in nature.



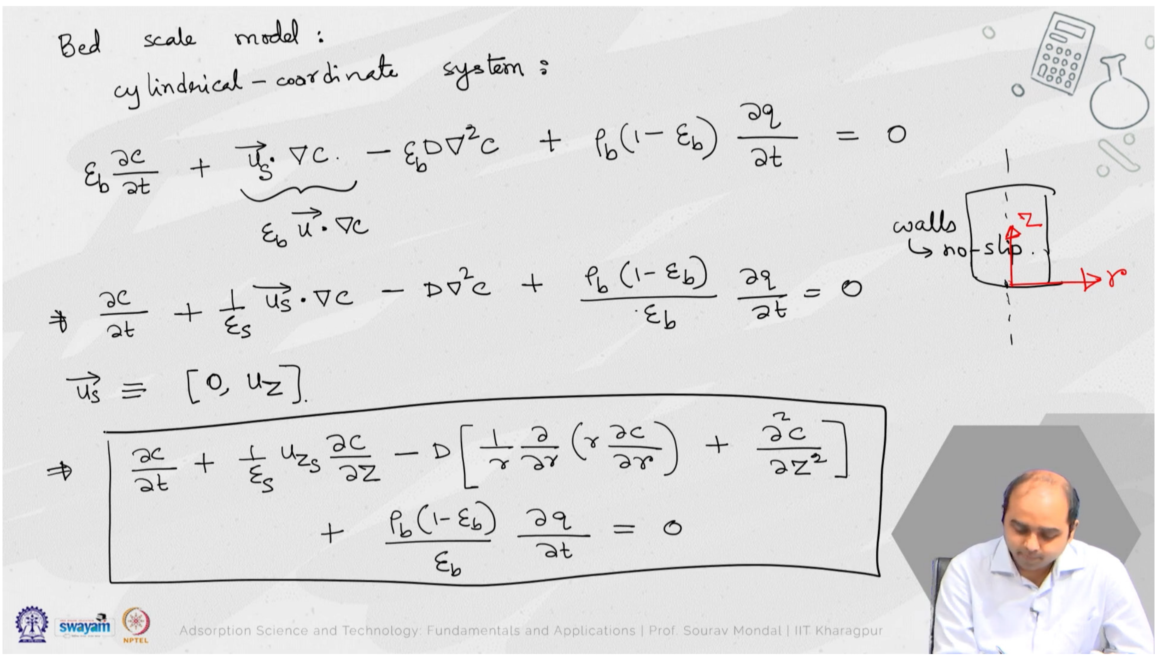
Now, this calls for a multiscale model. So, typically let me show you this schematic which gives a nice picture about how does a you know this adsorption bed can be considered. So, what I try to mean here is there is a you know concentration profile in across the axial direction and the radial direction with respect to time. So, there is a bed concentration or the concentration of the concentration of adsorbate at the bed level.

So, let us call that bed concentration as C bed which is a function of radius if the radius is significantly large and there is a radial effects. So, this r represents the radial coordinate of the bed z axial coordinate of the bed and time. So, this is the radial coordinate of the bed of the bed, z represents the axial coordinate of the bed. And at each location within this you know bed there is also something happening within the particles or within this adsorbent pellets. So, there is also an additional dimension to the problem with respect to the particle level or inside the particle concentration.

So, concentration inside the particle. Let us denote that as by Cp this is of course a function of the particle coordinate Rp. So, this is like the particle radial coordinate, and then it is also dependent on the location of that particle in the bed because the bed dynamics also influence the particle level concentration. So, that is why I also write these r and z and time because these coordinate locations as well as the time also influence the particle level concentration or exactly where this particle is located within my bed. The concentration of the adsorbate within inside of that particle will also be influenced by the its location within the bed and all of course, the particle coordinate assuming these are like all spherical coordinates the particle radial position or the radial coordinate inside this particle will also play a role.

Now, let us try to look into the macro scale or the bed level dynamics which is something that all is we have been discussing this so far. So, bed level dynamics So, if you consider a small you know control volume of delta r and delta z and then we can write the species transport equation as well as the this you know term related to this adsorption. So, let us try to write it down. So, we have you know this cylindrical coordinate system. So, here one can write this del c del t multiplied with the bed porosity I identify the bed porosity as epsilon b plus u where u is a vector u dot grad c this I consider to be superficial velocity.

So, there is no porosity term which is present there alternatively I can write in terms of this can also be written down as epsilon b u. instead of the superficial velocity minus D of grad square C. So, this is the diffusive term. This is equal to the rate of accumulation or you can also write the adsorption term here which is bed density, product of bed density with the bed porosity dq by dt. Now, here I do not consider that this dq/dt is actually something like the averaged particle concentration or at the surface concentration and that is something will be relating later on.

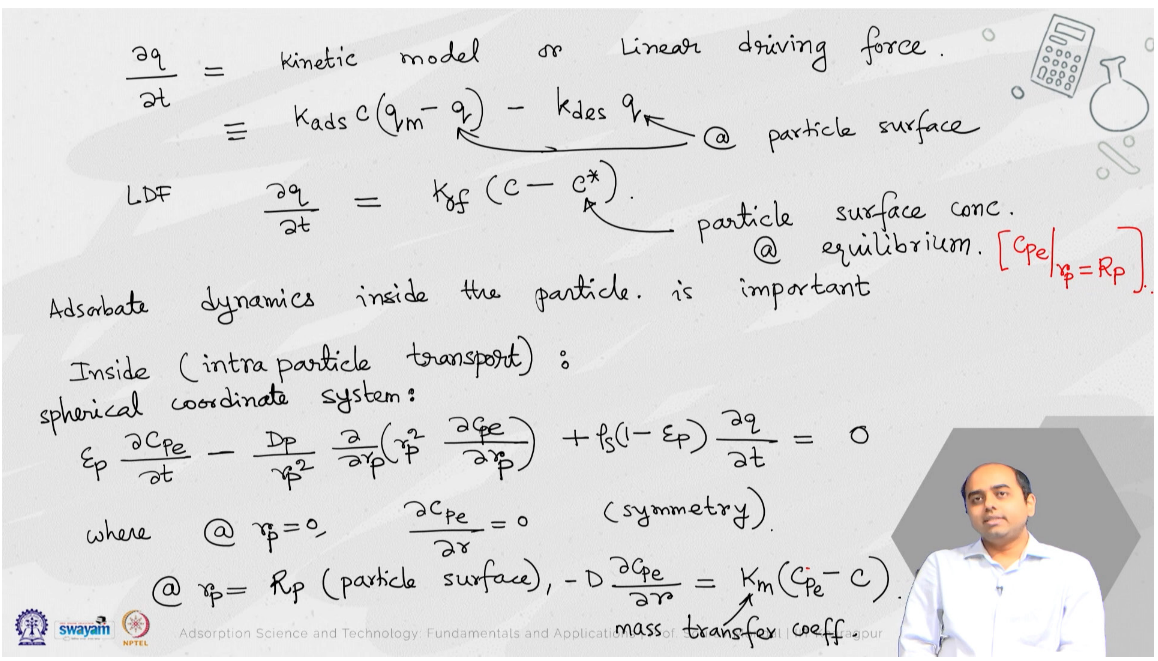


Now, this is the scenario here of course, the epsilon b would be also multiplied in before the diffusive term. So, if you are considering a superficial velocity then this equation can be rewritten as Now typically the convection along the radial direction is not present because the walls are of no slip. So if you consider a cylinder where the walls are no slip. There is no existence of the radial velocity. So, this u s or the superficial velocity vector is essentially u, sorry z comma 0 comma u z.

So, we are defining this as the z direction, this as the r direction. So, there are two components of the velocity u z and u r. This gets converted to u z S grad is. This term minus, generally the diffusion along the axial direction is very very small or very less compared to the radial direction, but this can also be true if the height of this column is not large. So, it is advisable that we write down the both the forms plus d 2 c by dz square plus rho b 1 minus epsilon b.

So, this is the you know bed level model or bed scale model. That is you know can be written down of course, taking into account of the diffusion and everything and taking into account of this bed porosity and everything. Now, coming to the aspect of dq by dt how one can find out what is the value of dq by dt. Now, to find out this dq by dt, it is essential that either we use the linear driving force model. So, dq by dt can be obtained from kinetic model or this linear driving force model.

So, in the case of the kinetic model we one can write this as K adsorption C q m minus q minus k desorption q. This is the Langmuir type kinetic model and particularly the concentration C here is relates to the bed concentration. Now, in the case of linear driving force model this dq/dt can be written down as an effective or overall mass transfer coefficient multiplied with C minus C star. So, this C star here is related to the particle surface concentration at equilibrium. Similarly, all of these values from the kinetic model this Q m minus Q or desorption into Q this of course, is based on the fact that equilibrium is not achieved or is not reached and this is the kinetic model in that case is very relevant.

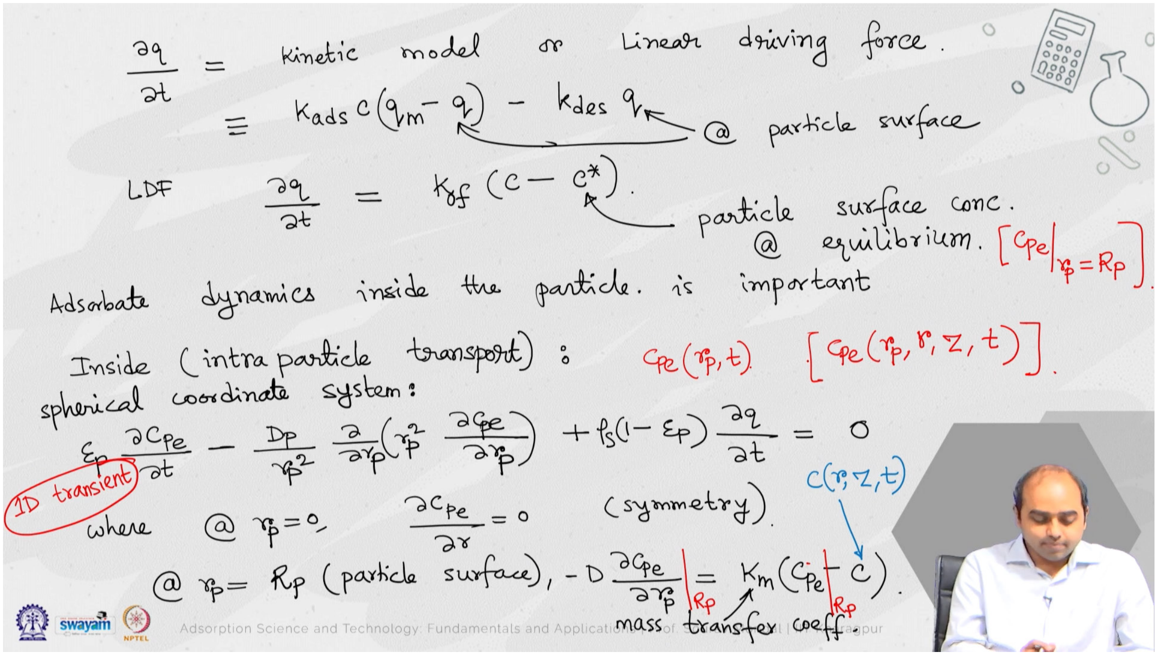


The Q in that case, is the value of the Q at the surface of the particle. So, whatever whether it is a linear driving force model or the kinetic model, in both of these scenarios it is essential to know because the Q in the kinetic model is at the the value of the Q or the adsorbate concentration at the particle surface. So, the particle level dynamics or this adsorbate dynamics inside the particle is important Now when it is not important when the Biot number of the system is large then we do not need to worry about what is happening inside this particle but in most cases that is not true. So adsorbate dynamics of course inside the particle has to be considered and to consider that adsorption dynamics inside the particle we have to use the transport equation within the particle. So now inside the particle, this is what is known as this intra particle transport.

One has to look into the picture. So, within the particle or inside of this particle, we will have the concentration is referred to as Cp or Pe within the particle. This would be multiplied with the particle porosity. Inside the particle there is no convection, so only diffusion.

This is like Dp. So this is the diffusion and we have the absorption like this, is a spherical particle. This equation of course is in spherical coordinates, where at r is equal to 0 del Cpe/del r is equal to 0 because of symmetry. The interesting question or the interesting point comes at the you know this at the particle surface at r is equal to sorry this is all rp so these are all particle coordinates not bed radial coordinates. So at rp is equal to capital Rp that is at the particle surface. This D flux boundary condition is satisfied there D of Cpe del R minus of that is equal to the surface mass transfer coefficient Kf is or I will write Km this is nothing but the mass transfer coefficient.

Cpe minus C where this Cepe at the surface will actually be linked. So this Cpe will be linked here. Cpe will be equal to Rp is equal to capital Rp. So, if it is I mean it is already assumed or it can be easily assumed that you know this adsorption kinetics is fast compared to the diffusion time scale. In that case the particle surface concentration would reach equilibrium.



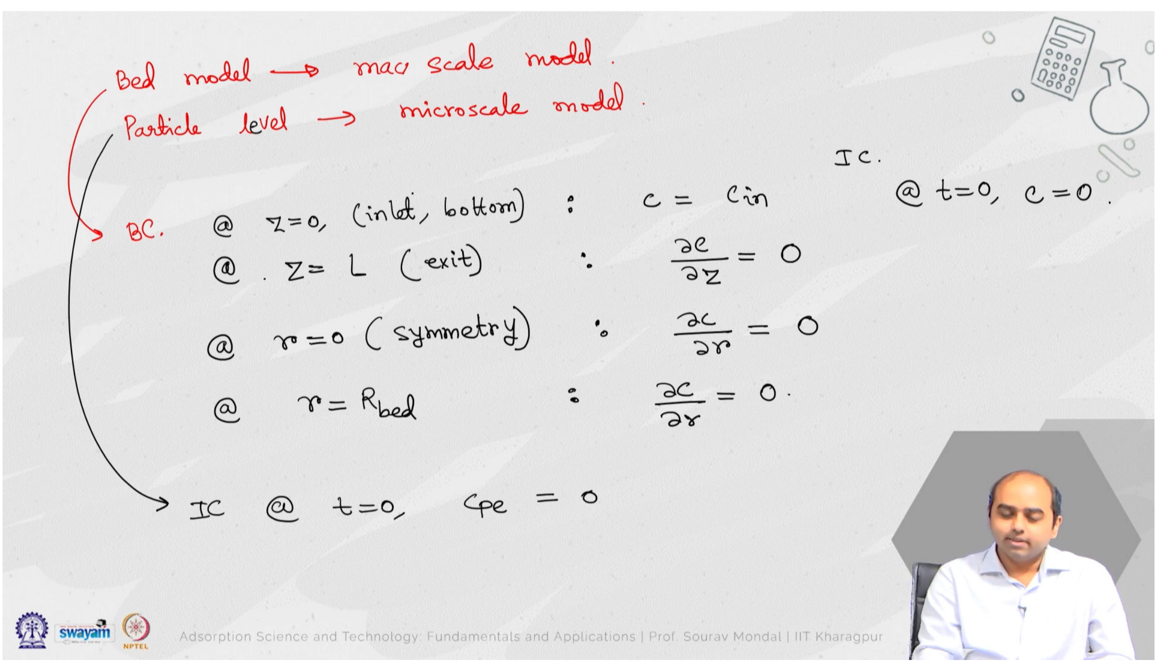
So, in that scenario or the particle concentration at the surface would be much higher or will be at the equilibrium concentration. In that case, these from the intra particle analysis one would get the value of particle surface concentration. So, this is at Rp, this is at Rp and that will be fed into the main either the linear driving force model or the whatever the other types of model can be fed into this main equation or into the bed scale equation. Now, interestingly this problem is coupled at r is equal to Rp because the value at r is equal to Rp is essentially not known a priori to the solution either solving the you know bed scale equation or solving the you know this particle level equation. Because to solve the bed scale equation this quantity this dq/dt is to be obtained from particle surface.

So, as you can see this bed equation is 2 dimensional in its nature 2 d transient, but since the, since the particle surface and to evaluate the particle concentrations, we also need to know the value of C from the bulk. So, this quantity C is essentially the concentration of the solute in the bulk. So, this C can be written down as C as a function of the bed scale coordinates and time. So, this is where the problem is coupled in this case and is referred to as the multi scale model. So, this boundary condition or this flux boundary condition is coupled with the value of the bed scale model feeding into this problem and hence the solution of this intra particle transport is also linked through this boundary at the particle surface to the bed scale equation.

Although the particle level equation is one dimensional in time, so this is 1D transient equation, it still since it needs information of the bed coordinates of the radial and the axial coordinates, this problem Cp. So, even though Cp appearing from this equation is only a function Rp and time but in reality that is not true because Cp or this particle concentration is essentially a function of the particle radius and the bed radial and the axial coordinates and time. So, this concentration profile within the particle is actually like an extra dimension to this problem. Now coming to the overall picture this for the so, the bed model is essentially the macro scale macro scale model this particle level model, is the micro scale model. Now, to solve this macro scale model we need to define the boundary conditions.

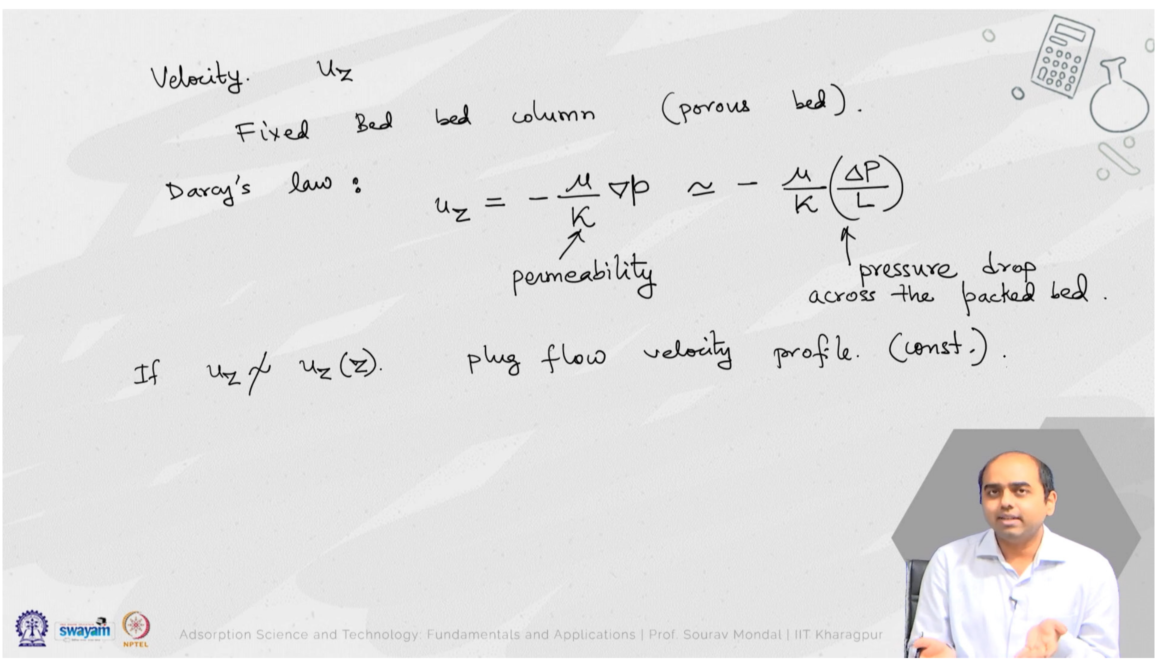
So, for the macro scale models the boundary conditions would be at z is equal to 0 that is like the inlet bottom. C is equal to cin at z is equal to l that is the exit or the outlet we define no flux condition or the far field boundary condition at r is equal to 0 which is like the symmetry boundary condition This problem is second order in R and second order in Z because of the diffusion terms in both in R and Z. This is like the radius of the bed. Again del C/del r is equal to 0. At the particle level also we have the initial conditions.

At t is equal to 0, C is equal to 0. At the particle level it is very important to define already we have defined the two boundary conditions at the particle level. So, the initial condition at the particle level is at t is equal to 0, Cpe is equal to 0. Now one thing we have not mentioned is inside the particles, inside these particle where does this you know this isotherm come in the picture and that is particularly very relevant. So, this isotherm is actually you know you know connected into the particle.



So, this qp, qp is essentially this q by q t is essentially at the inside of this particle. So, this is connected to the to the kinetic expressions, or mass transfer limiting dynamics. This is something which we have discussed in great detail in the previous week about how the inside the particle what are the different types of diffusion or the mass transport phenomena or if the kinetics is important then how does kinetics play a role and that is how it will be connected to dq or del q del t. Coming to the velocity, so this velocity in this at fixed bed velocity u z. So, this is a fixed bed column fixed bed column which is nothing, but a porous bed.

So, one can use Darcy's law. So, from the Darcy's law this uz can be represented as minus 1 by this sorry mu by the permeability mu by this is kappa permeability grad p. So, for simple you know since the for pressure driven flow this and as you considering that constant pressure drop is there this can be related to delta P by L. Pressure drop across the packed bed. Of course, in this if you consider the pressure drop to be constant throughout the bed, then in that case Uz becomes a constant or this flow becomes a plug flow type. But if that is not the case, for example, in the case of gravity driven flow, So, this pressure drop is sorry pressure drop is of course constant, but if you want to calculate this you know pressure drop at different heights and this Uz is not constant or if the pressure drop is not constant.



And, then in that case this uz becomes a function of z particularly in situations where you know where the Froude number says larger than 1 or where the role of gravity is become significantly higher. In that case the case of the Darcy law suggest that u z becomes a function of z. So, if u z is a function of z is not a function of z then you get the plug flow velocity profile or constant velocity can be constant, which is generally the case because pressure drops are generally not varying unless this is a very big column or something or wide diameter pressure drops generally constant and this u is not a function of z. But nevertheless it is important to that we know the how it is related or how it can be calculated from the Darcy's law. So, with this I consider that you know all of you have a fair understanding of the multiscale nature of this bed and how these two concentration at the particle level and at the bed level are connected.

And this becomes particularly important when the intra vertical dynamics cannot be considered as like an equivalent or an averaged adsorbate concentration which is something that we do for, I have done already or explained for previous scenarios, but instead we try to account for the intra particle dynamics or diffusion inside the particles plays a big role in such scenarios the intra particle effects need to be essentially considered and the problem becomes multi scale in nature. Thank you. In the next class we will talk about some example and illustrative problem using the methods that we have discussed already in the last week. And following which we will be talking about pressure swing adsorption which is a specific example of fixed bed adsorption column and its application and use in practical as life as well as industry. I hope all of you found this insightful and interesting. See you everyone in the next class.