Course: Adsorption Science and Technology: Fundamentals and Applications

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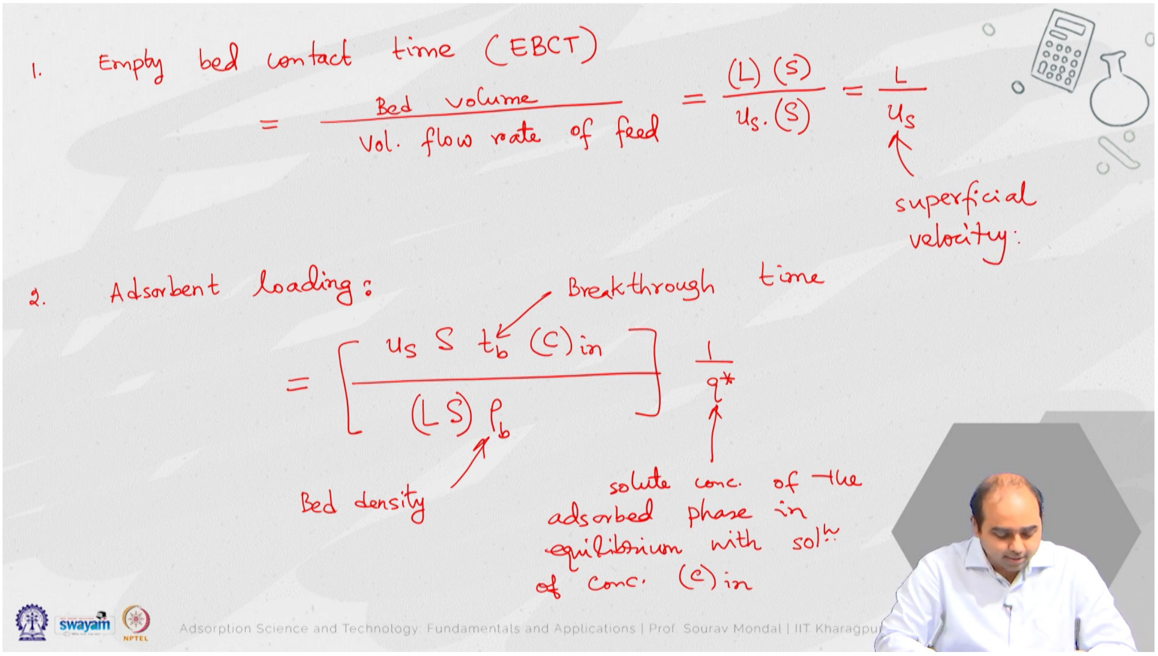
Week 05

Lecture 23 | Fixed Bed Design: Thomas Model

Hello everyone, welcome to this class on adsorption science and technology. So, today we are going to talk about some of the you know models today and in the next few classes regarding fixed bed adsorber modeling. So, today I have planned to talk about this famous you know Thomas model, why I say famous is because it is particularly very popular in modeling you know fixed bed designs and you know upscaling of the fixed bed with certain simplifications of course, which we going to look into it, but this gives a reasonably accurate solution to the you know this transport problem involving adsorption. Now, before we go into the details of the Thomas algorithm, I just want to quickly introduce you know few terminologies which is very relevant in this fixed bed adsorption modelling. The first one is the is known as this empty bed contact time, popularly represented as EBCT. Now, this contact time is actually the ratio of the bed volume divided by the volumetric flow rate of feed.

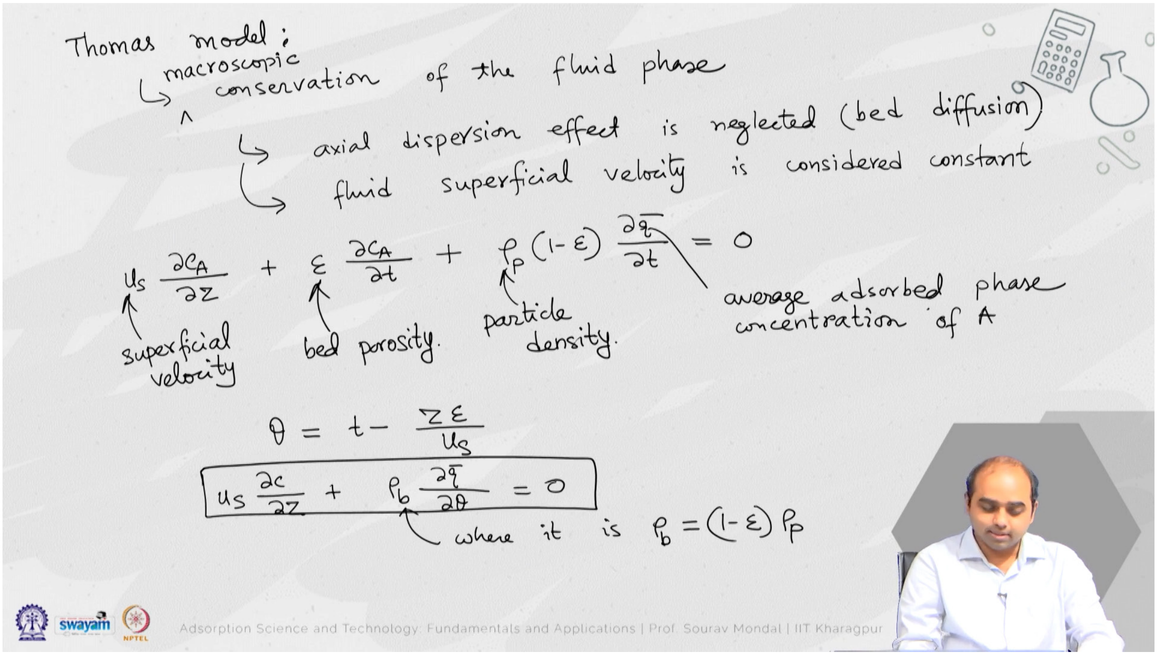
So, this can also be written down as you know the length of the column, the surface area of the column divided by the linear velocity, superficial velocity with the cross section of the column. So, this turns out to be the length of the column divided by the superficial velocity provided the area of cross section is same throughout the column. So, next important terminology which is often referred to is the adsorbent loading. So, this actually provides information about the efficiency of the adsorbent usage in the fixed bed and often represented as a fraction of the saturation capacity of the bed.



So, this is represented as the total amount of the you know this adsorbate which is absorbed in the bed. So, t b is the breakthrough time and C in is the inlet concentration divided by the volume of the bed multiplied with the bed density. This whole divided by 1 by Q* where essentially Q* is the solute concentration, of the adsorbed phase in equilibrium with solution of concentration of the inlet solute at the inlet condition. Of course, rho b represents the bed density, tb represents the breakthrough time and Us represents the superficial velocity. So, now let us look into the Thomas model.

So, in the Thomas model what is essentially done or this model is all about it is a conservation or let us call it as macroscopic conservation of the fluid phase. Now, this is important to note that there are certain assumptions which is inherent or implied in the Thomas model. So, that is why this solution can be often referred to as sort of the approximate solution. So, these assumptions are that this axial dispersion of solute is neglected. Another thing is the fluid superficial velocity is considered.

So, with these two assumptions, we can write the, you know, this macroscopic balance equation as like this. So, the Thomas model is essentially a macroscopic balance of the fluid flow the fluid phase system and this is involves you know two important assumptions that I have already noted it down. So, the macroscopic you know conservation equation is what something I have written it down here. So, please note that here the this U s represents the superficial velocity and this q represents the average absorbed phase concentration of solute A and rho p of course denotes the particle density. epsilon represents the bed porosity.



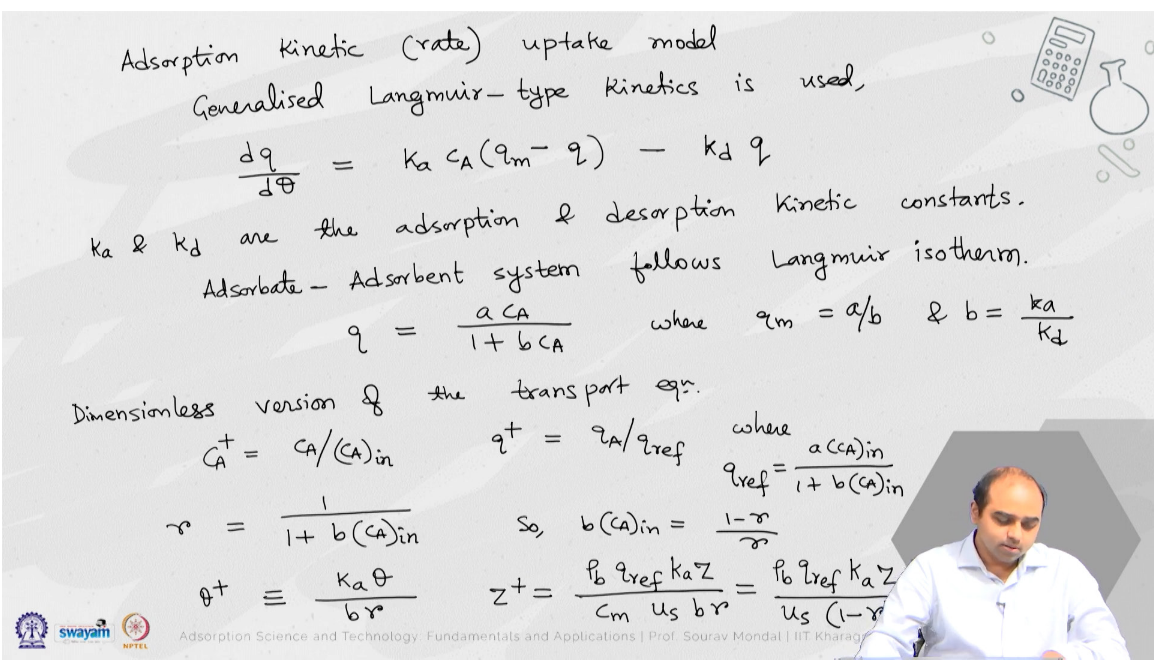
So, in this case if we try to modify this equation by defining a new time theta which is equal to which could be equal to t minus z epsilon by us. So, this theta is like defining the characteristic you know time in this case and we are subtracting the you know physical time here with this characteristic time this is also related to the empty bed contact time at that particular value of the z or this adsorption wave front present at z. So, doing this transformation considering theta to be like t minus of this the above equation the conservation equation does get modified to something like this. where of course we write this where it is this bed porosity is 1 minus epsilon of the particle porosity. So, this is the simplified you know version of this equation considering this constant wave pattern in this case or when there is absolutely no axial dispersion or there is you know no effect of the diffusion of this solute.

So, diffusive behavior, this bed diffusion is also neglected in this case. So, the motion of the solute or the fluid flow within the porous bed is purely convective in nature. In that circumstances the you know the solution can be obtained with the help of method of characteristics and this is what the characteristic time is defined or scaled appropriately here. Now, with this transformation it is important to identify that what would be the value of dq/dt or dq/d theta in this case or the averaged adsorbed average adsorbed phase concentration in this scenario. Now, typically this is given by the adsorption kinetic rate uptake and the Langmuir type generalized Langmuir type kinetic is used here.

d qs / dt or d theta can be represented something like this. Where of course, Ka and Kd are the adsorption and desorption kinetic constants. So, this also suggest that since this is given by the kinetic expression, this adsorbate adsorbate system follows Langmuir isotherm or Langmuir equilibrium isotherm which is nothing but q is equal to a CA by 1 plus b CA where qm is a by b and b represents the ratio of the forward to the backward uptake rate expressions. So, this is the you know this dq by dt is used from the kinetic expression. It is also possible to use there is an extension to this Thomas algorithm.

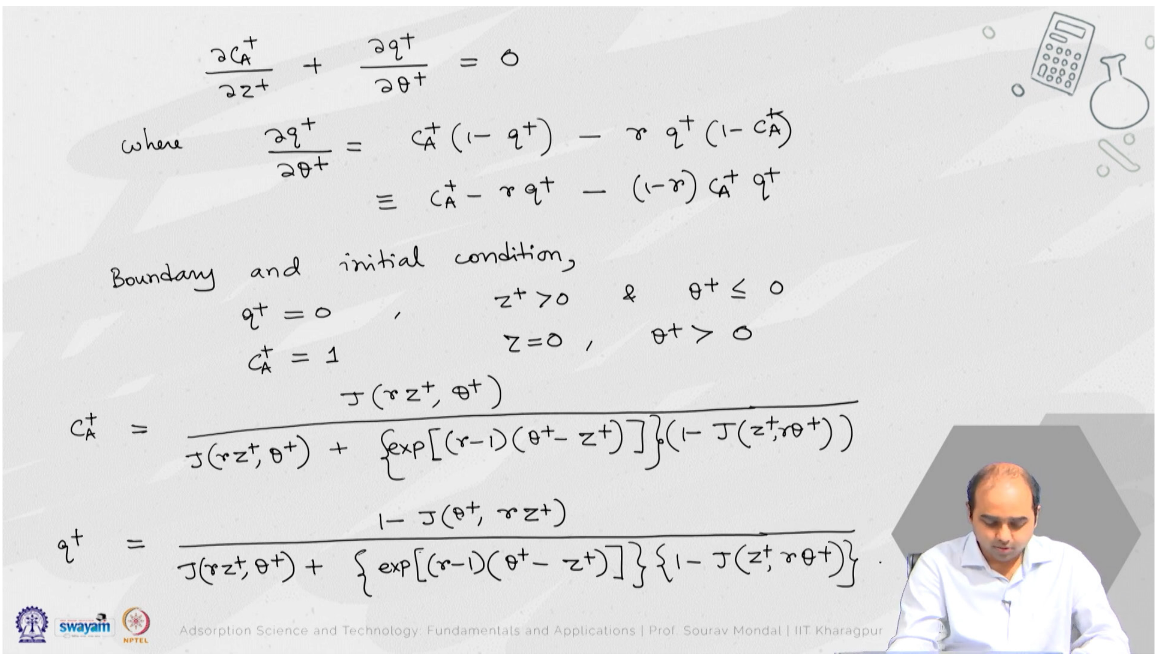
It is also possible to use the sort of the linear driving force or the mass transport based relation for dq/dt particularly when the kinetics is fast in the process, but the analysis method remains more or less the same. Now, we write down the dimensionless version of the transport equation. So, I am talking about this expression which we are trying to write down the dimensionless version. So, I will define the dimensionless version or the dimensionless quantities as with a you know positive plus symbol at the superscript. We also define some other additional variables as this.

We define a non-dimensional scaled time as something like this. Define a scaled coordinate. So, this is nothing but equal to. So with these you know conversions or scaled parameter this transport equation can be written down as. So where dq plus d theta plus can be written down as c a plus 1 minus q plus so which is nothing but equal to c a plus minus r u plus the boundary conditions and the initial conditions which are defined as.



So, this is a. This is the first order in Z and first order in time. And at the inlet we define this as 1. So, we say that initially the bed is completely unsaturated there is no solute or no adsorbate and at the inlet we define the concentration CA is equal to 1. So, in this case the solution of this equation is given in this form for both CA and qA.

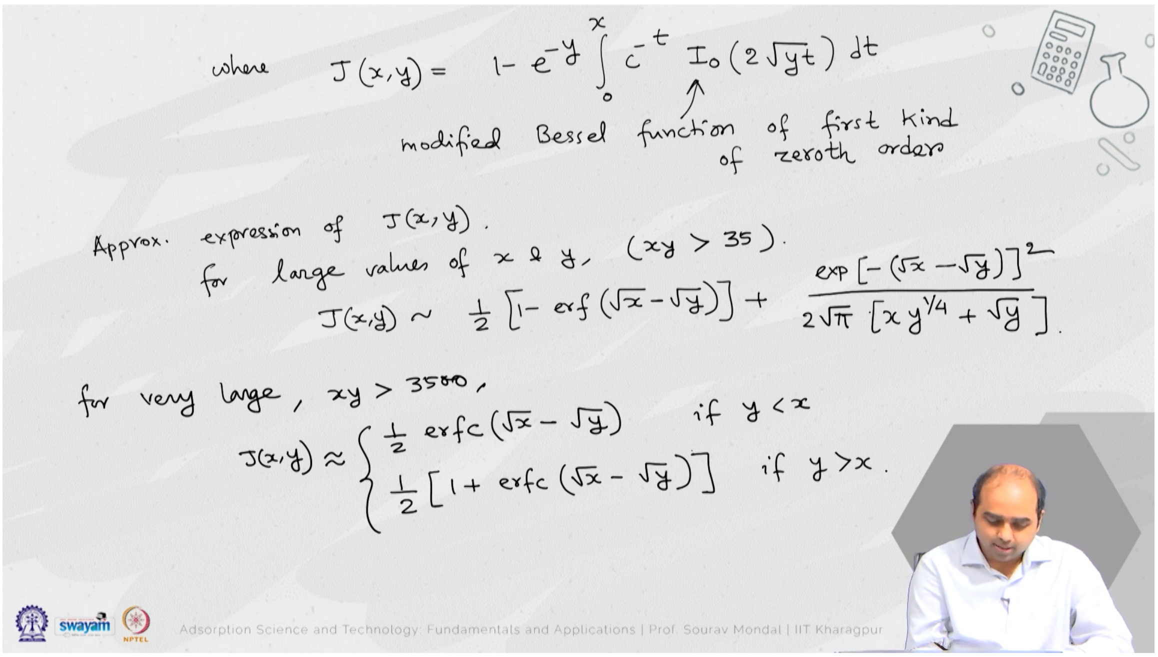
So, I will write. So, please note the J here does not represents the Bessel function and I will define what does this J mean. So this is what CA+ looks like. For q+ the solution looks because c and q are related. So, finding out one can also help in finding out the other. The denominator essentially stays the same.



Now where it is important to define the function J. So, this J x comma y is defined as 1 minus exp(-y), 0 to x and here I0 represents the modified best Bessel function of first kind of zeroth order. So, here I0 represents the modified Bessel function of first kind of zeroth order. So of course there are some properties which I can say, share with you here. Like the approximate, approximate expression of J(x,y).

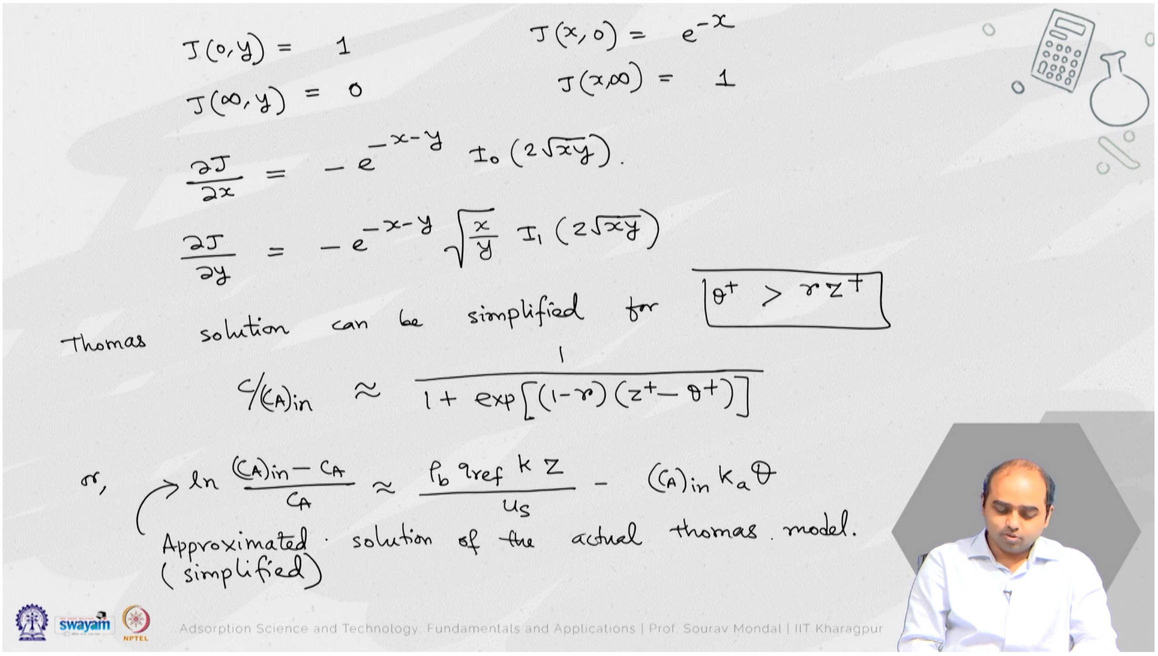
So for x y are large values, for large values of x and y, this J(x,y) of is simplified like this with the help of the complementary error function. So, this is the scenario when x, y is large and when it is very large. So this is particularly for the scenario when x by y is like greater than 35 or so. When it is very large, so which means x when y is like much greater than 3500. This is represented as, this is the complementary error function.

if y is less than x and if it is greater than x then this is the relation. So, now it is very important I mean all of you must have realized that this expression of the this J is very important in the evaluation of this entire thing. Some of the limiting values also I must mention like for example J of 0 comma y if x is 0, then this turns out to be 1. J of x comma 0 gets converted to e to the power minus x. J of infinity comma y is equal to 0.



J of x comma infinity is equal to 1. And of course, derivatives and some things can also be defined. So, for example, dJ/dx can be defined as minus e to the power minus x minus y, I0 2 root over x y. Similarly, dJ/dy can be written down as minus e to the power.

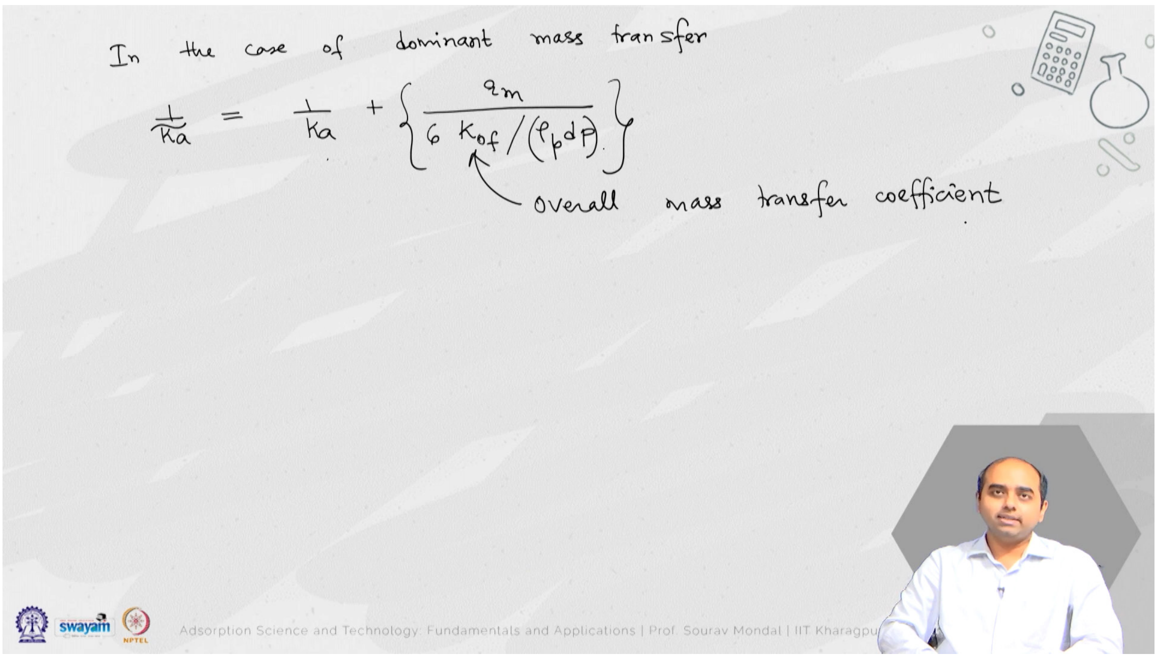
It is like this. where I1 and 0 represents the modified Bessel functions of zeroth or first kind of zeroth and first order. Now, this can be the solution of this Thomas algorithm can be simplified you know for theta for this Thomas solution. can be simplified for situations when theta plus is greater than r into z. So, in that scenario this entire solution takes of this form which is something all of us are used to in you know as the name of the Thomas algorithm. But please note that this only exists under this assumption.



So, this can also be modified as ln of, if you take the logarithmic values on both sides this represents. Thank you. So, this as you can see is the classical you know this expression of the Thomas algorithm sorry as the Thomas solution for fixed bed adsorption model particularly where C is you know mentioned or C is actually denoted as a function of this Z in this scenario. So, this is the approximated solution this is the approximated solution of the actual how much you know model. that we have represents and that is normally used since this criteria of theta greater than R z is valid in most practical scenarios.

So, I would like to quickly also talk about regarding the extension of the Thomas algorithm to include mass transfer effect. So, in the case of dominant mass transfer instead of the, you know, this kinetic rate expression, one can also use the expression from the, this mass transfer. So, something like 1 by Ka for this modified constant I write 1 by ka. So this is sum of the resistances. So, as you can see or as you can note that in this case the this modified adsorption rate does include the adsorption constant as well as the contribution or the relative contribution from the you know this mass transport effect based on the linear driving force law.

So, particularly this Kof is the overall mass transfer coefficient in this case. Of course, further resistances this is mostly the mass transfer resistance due to the adsorption inside the particle phase. Of course, there could be some additional mass transfer resistances in the during diffusion in the fixed bed. The adsorption kinetic constant may be you know smaller or larger than the this mass transfer resistance or the resistance due to this kinetics can be you know smaller in that case this coefficient Ka or this mass transport based model is this entire Thomas algorithm, Thomas solution or the Thomas method of the solution becomes further simplified when the Langmuir based kinetics is actually replaced with the dominant mass transfer. But there is one catch and something that I would like to essentially mention that the kinetic constants used in the Langmuir isotherm is can be replaced with the constants from the mass transfer coefficient theory in this case.



And this can be considered as to be the sort of the pseudo you know reaction rate constant or something like the overall rate coefficients in this scenario. So, with this I would like to close the lecture on Thomas solution or the Thomas model. In the next class we are going to talk about certain simplifying scenarios of the Thomas model and we see that how the other different types of model actually emerge from this simplifications. I hope all of you found this lecture useful.