Course: Adsorption Science and Technology: Fundamentals and Applications

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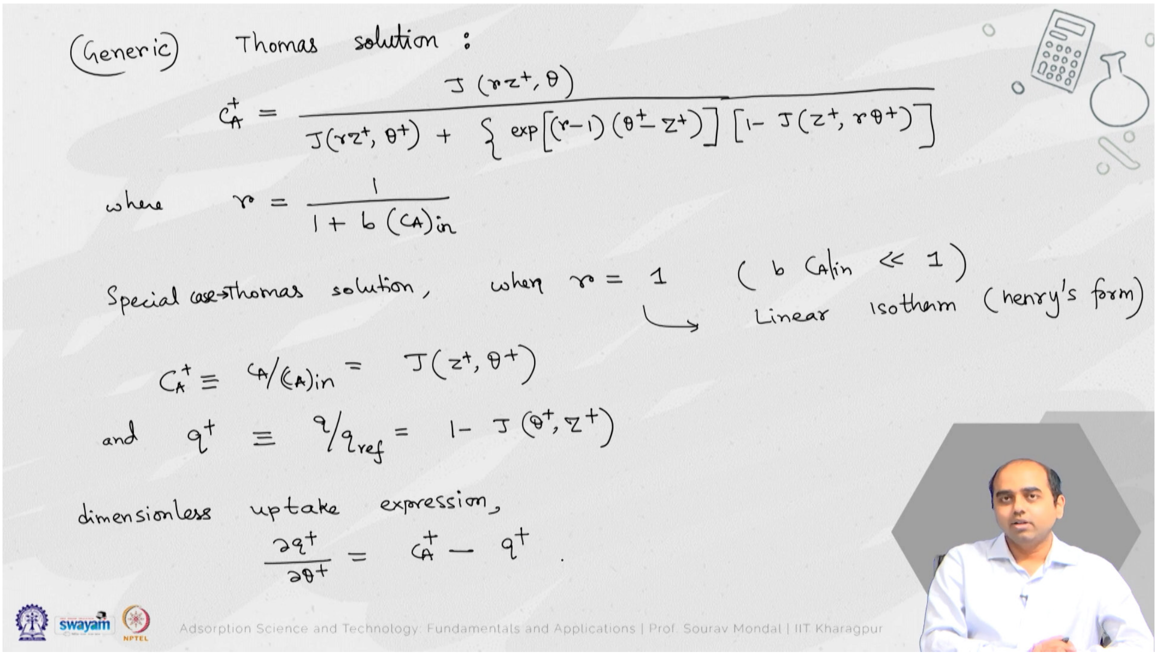
Week 05

Lecture 24 | Fixed Bed Design: Adams-Bohart and Other Models

Hello everyone, in this lecture we are going to talk about the different you know simplifications of the Thomas model in itself and how that you know develops the other models that we often refer to particularly for fixed bed adsorption design. So, in this lecture we are going to talk about primarily the Adams-Bohart and we will see how that is derived from the Thomas relation as well as some other you know this bed design models. So, first just a quick recap on the this adsorption model solution based on the Thomas model. So, if you recall the Thomas model in the last lecture we have already written down the solution in terms of this J. So, the generic Thomas solution, for the bed design is given as like this. Now, here the important factor or the parameter is this r.

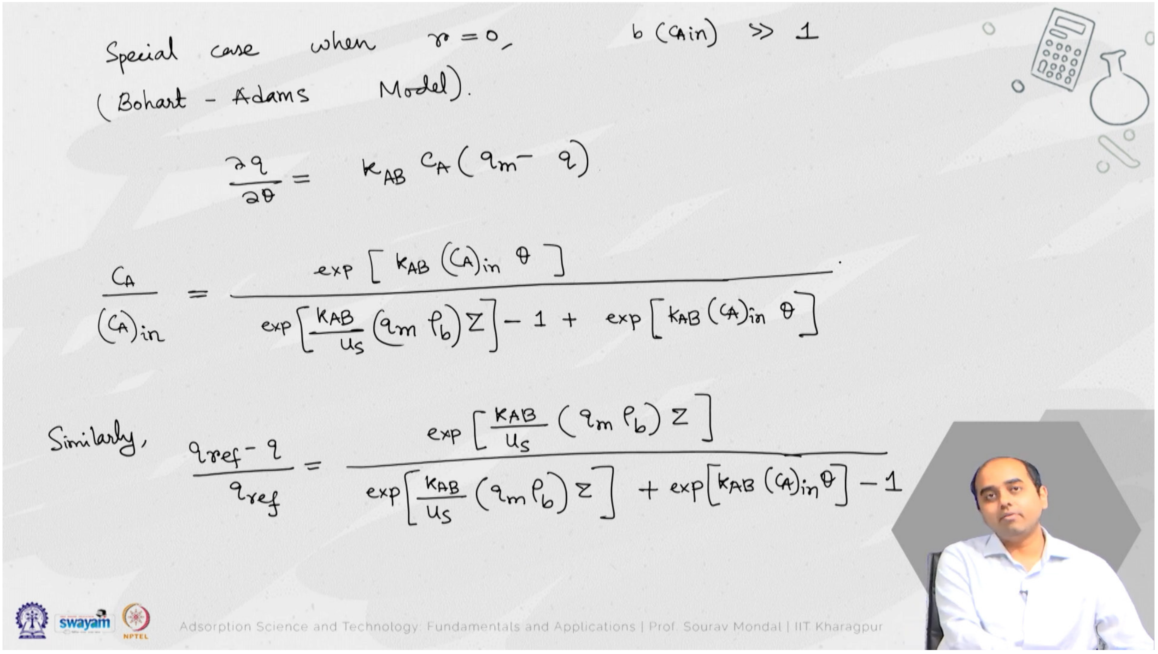
So, this r is defined as something like this of course, the this represents the denominator of the Langmuir isotherm kinetic. Now, the first you know simplification or the special case I would say of this how much solution is when r is equal to 1. So, the when r is equal to 1 it suggest that this b by c a in or denominator or this particular this value of the b is much smaller. So, when r is possible when b of c a in is much much smaller than n.

So, in this case the Langmuir kinetics you know this or the Langmuir isotherm generally gets converted to the scenario of linear isotherm something like the Henry's form. So, in this scenario when r is equal to 1 the solution of CA plus which is nothing but CA by CA in is simply J of z plus comma theta plus and Q is which is nothing but Q by Q ref is equal to 1 minus j of theta plus comma z plus. So, this is the simplified solution when r is equal to 1, and of course, the dimensionless uptake expression can be written down as something like this. Now, it is important to realize that this is a simplification or let us say a special case of the Thomas solution particularly for linear isotherm models or particularly for low concentrations of the Thomas solution where the isotherm equation only follows a linear behaviour particularly at the low range of the uptake or the isotherm profile the Thomas solution can be simplified into this form. Now let us look into the situation of the second case which is particularly very interesting.

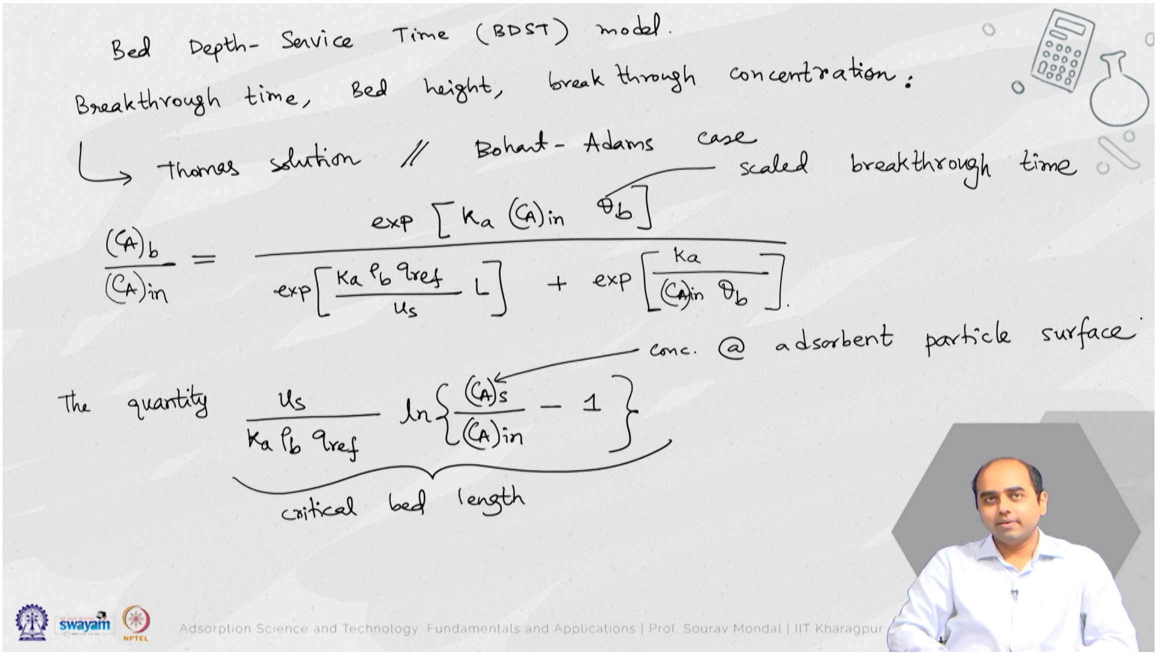


Now another special case is r is equal to 0. This is the scenario when b of CAin is much much larger than 1. So, it is in this limit this you know this r can be equal to 0 or this is the zone when the adsorption actually reaches close to saturation. So, this model or this reference is known as this Bohart-Adams. Many people also do call as Adams-Bohart model.

And we will see that the expression of the fixed bed or this Thomas system is at least the kinetics gets converted to this form. I will write as Adams-Bohart or Bohart-Adams kAB this constant, CA qm minus Q. And in this case that for fixed beds you know adsorption with fresh adsorption adsorbent and constant influent concentration CA in that you know whatever the solution that you obtained for the Thomas model can be simplified. And one can get a solution of this form. So, please this AB and BA are essentially same.

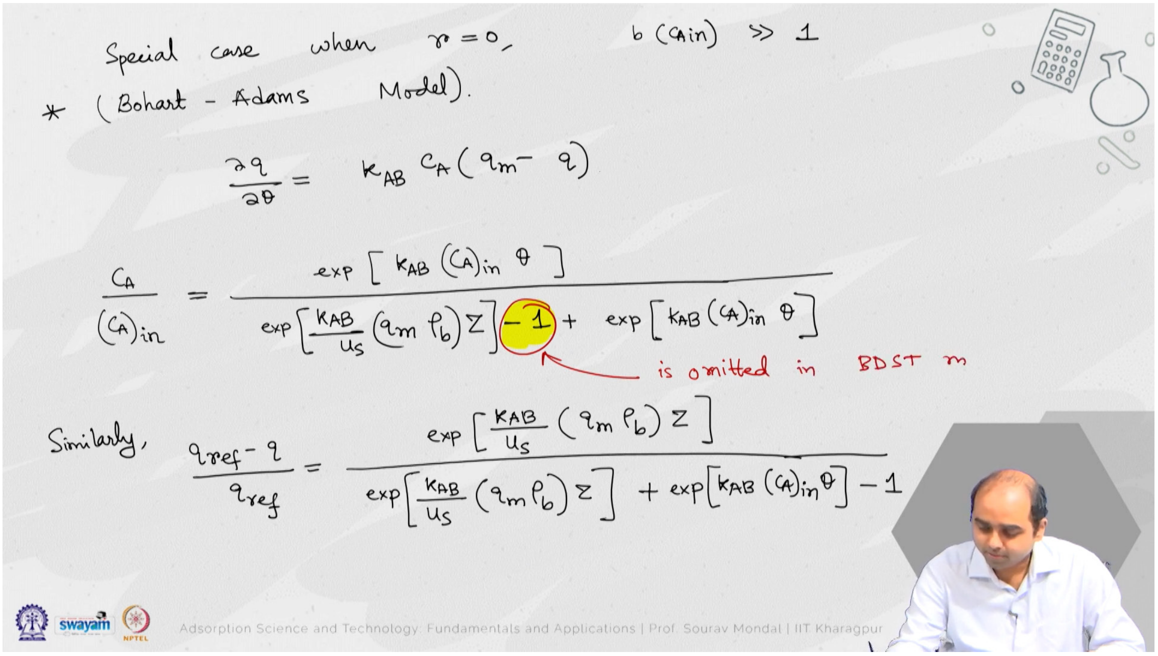


I mean I should write all as AB. So I am writing everything in dimensional form and this is something that you can obtain also from substituting the different dimensional version of the dimensionless quantities. Similarly Q solution. So, these are the two you know equations or the two form of the equation which primarily you know represents the Adams-Bohart or the Bohart-Adams model solution where the concentration profiles or the with respect to Z, can be tracked and this is something is useful in the model of this you know this breakthrough curves as well as to determine the length or the height of the adsorption column under these circumstances, where it is not feasible to solve for the entire you know actual solution which is something we will of course talk about in the next lecture. But this in this scenario this is what you know a simplified version which of course comes from the Thomas solution can be presented and this represents this Bohart model or this Adams-Bohart model.

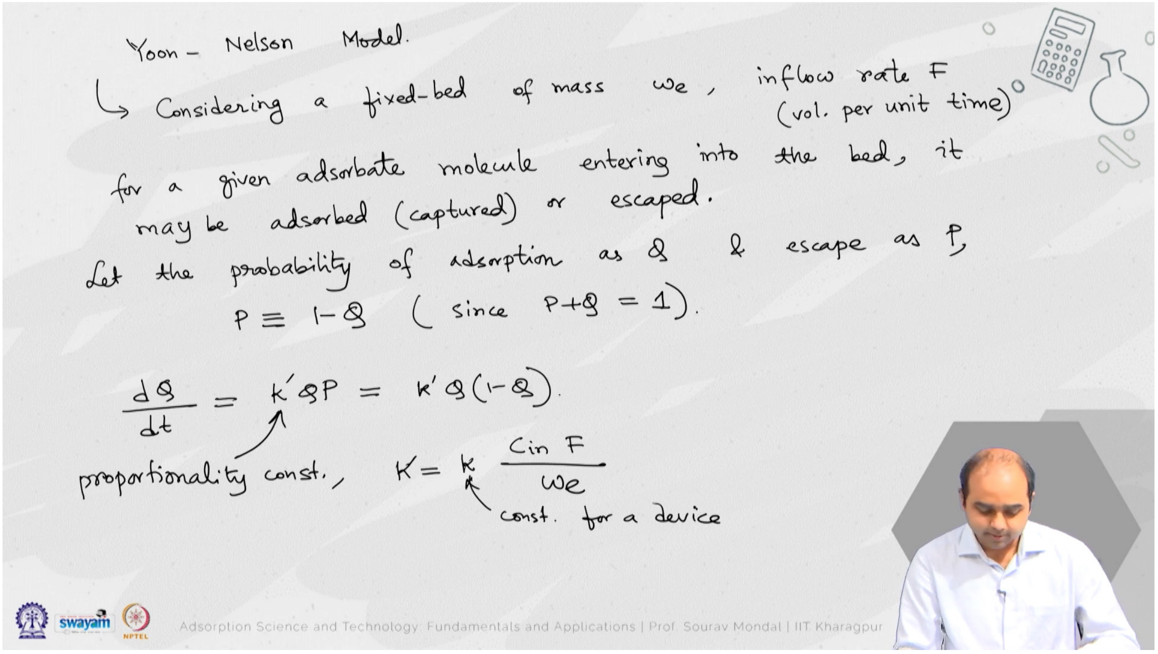


I would like to emphasize here one particular thing that in the absence many a times there is another model which is you know generally referred to as in and in connection to this Adams-Bohart model is the bed depth service time or this BDST model as it is popularly known as. This is again the solution of the approximate Thomas model and this is something can be used to relate the breakthrough time, bed height breakthrough concentration. And this is actually originates from the Thomas solution particularly the Adams-Bohart case and here this is written as the value at the end or when Z is equal to L. So, CAb represents the breakthrough concentration. So, in all of these expressions I hope all of you notify the I mean note that the ratio of L by uS comes in the picture which is nothing but the empty bed contact time.

Not only that, this quantity, the entire quantity within this expression K a rho b q reference into L also can be related to the relative adsorbent loading as there is something that we have defined in the beginning of the previous class. Of course, you must, one must understand that there exists a linear relationship between this theta b or this breakthrough time. So theta b represents the scaled breakthrough time and it is related to the length of the absorber, particularly the quantity in this case Us by ka rho b q reference. This quantity refines the you know critical bed length which is like the minimum bed length for the fixed bed adsorption column to essentially function properly. So, this is the concentration at adsorbent particle surface.



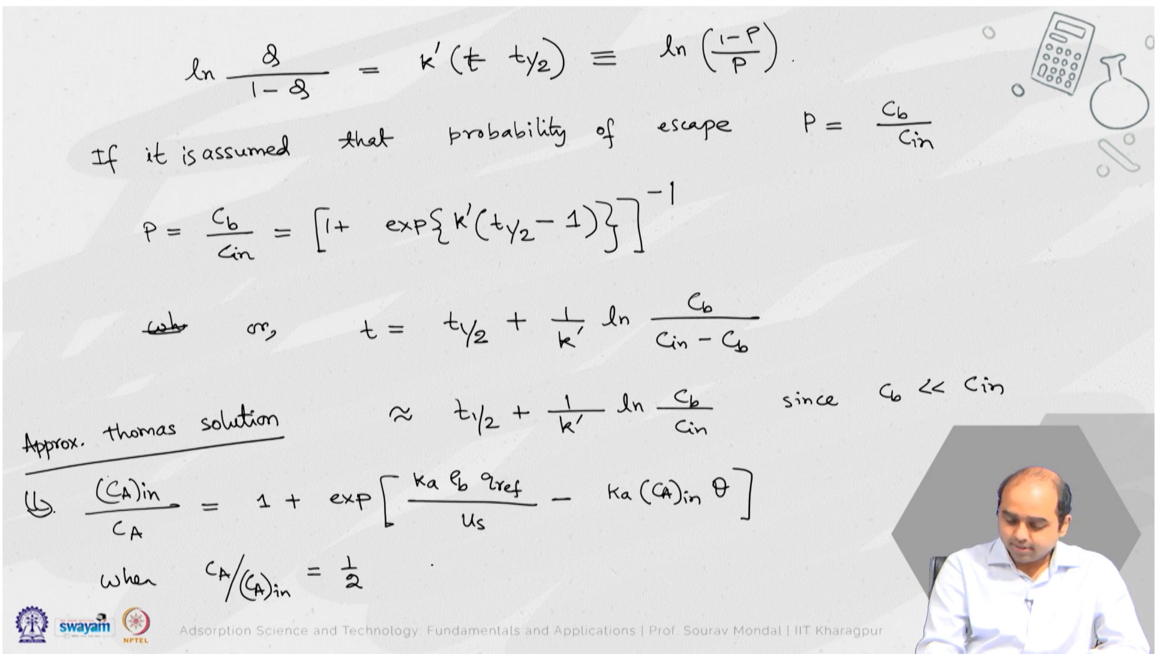
So, if you note carefully here this bed depth service time service time BDST model is almost I would I am saying almost because it is closely similar to the this Adams-Bohart model just one exception that here in this case the value sorry this denominator 1, is actually removed in this expression from this relation in the case of the. So, this highlighted zone part this 1 from denominator is omitted in this bed depth service time model. Next, there is another sort of semi-empirical or I would say an empirical model which exist and we should talk about that as it is also particularly popular known as this. So, these are all simplified scenarios or simplified cases, Yoon-Nelson model, these are based on simple rate uptake expressions. So, here you can consider the basis of this model is that considering a fixed bed of mass let us say w_e and inflow rate F for a given adsorbate molecule entering into the bed, it may be adsorbed which is like captured or escaped.



So, let the if we define the probability of adsorption as Q and escape as P, then one can define P as 1 plus Q since P plus Q is equal to 1. So, change of Q with time in this case can be related by this simple rate expression something like this where of course, this is a proportionality or rate constant let us say proportionality constant. So, change of Q with time in this case can be related by this simple rate expression something like this where of course, this is a proportionality or rate constant let us say proportionality constant. So this rate of this you know capture or this rate of adsorption is proportional to the probability of adsorption and the probability of escape equally that is how we wrote this and the proportionality constant is k prime and this is nothing but equal to k prime. This k prime or this proportionality constant can be referred to as this and multiplied with a k which is like a constant for a device.

So, with this basis the solution can be related to ln of Q by 1 minus Q like k prime t minus t half which is also equal to ln of 1 minus P by P. Now with this idea if it is assumed there is a lot of assumption but please try to understand the assumptions. It is assumed that probability of escape this P is equal to this breakthrough concentration with and the relative breakthrough concentration with respect to the inlet concentration. Then one can get the expression as where of course, t half represents the half life, as minus 1 or this can be written down in terms of t is equal to t half plus 1 by a prime ln Cb by Cin minus Cb. So, in most cases since so this can be further approximated as this.

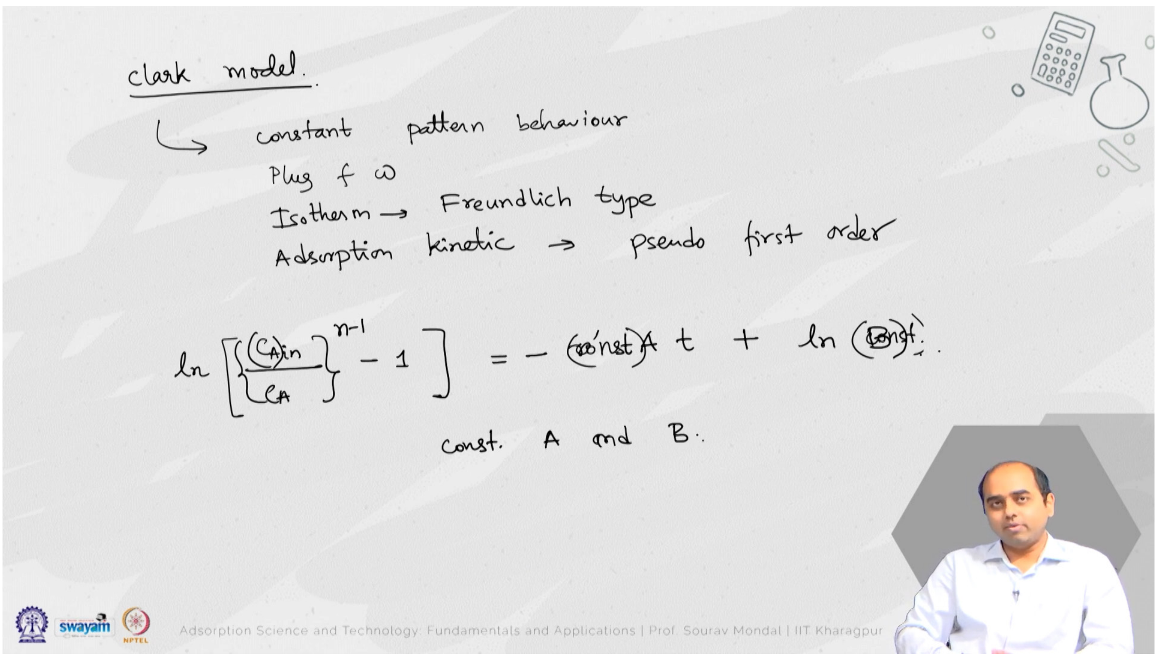
Since unless it reaches through you know this concentration close to the breakthrough this can be written down as a simplified version in this case. So, one of the surprising feature of this model is that you will note you might have noticed is the omission of the bed height effect. So, while this omission may be accepted for shallow or small bed heights in the case of you know small systems for example, oxygenators, this household respirators, it is used in fixed bed where the bed size is significantly longer questionable. So, it can also be written down this model can also be written down in terms of the approximate version of the you know Thomas solution very similar to the Adams-Bohart model. So, in this case this will appear as.



So this is the approximate Thomas solution. So when this C by CA in is half. So, this is the scenario which suggest that t is equal to t half. So, from this you know above expression one can find out that for this case 2 is equal to 1 plus exponential a rho b q ref by us z minus k a. This is the expression of theta half and from here theta half is rho b q f Z by U S.

So, this gives us an expression about how does you know theta half would look like. So, putting this expression you know back into the solution you I mean theta half can also be used to work out what would be the t half expression. So, this is about the Nelson model. So, this particularly involves the probabilities and it use I mean this is sort of a this you know argument of the that comes into the picture with respect to the this constant based on the probability of the adsorbate and the adsorbate getting adsorbed as well as getting escaped. So, there is one or two more models.

One more model I will particularly discuss here is the Clark model. So, in the Clark model, this is also based on the constant pattern behaviour which will something discuss in the next lecture in detail. Plug flow type, plug flow then isotherm is Prandtl witch type and adsorption kinetic is pseudo first order. So, this model the I mean this is something a slightly modified version of the Yoon-Nelson model where instead of using the Langmuir idea you use the Freundlich idea. So, this looks where n is the exponent of the, you know, Freundlich isotherm.



So, there is one this constant. I will write a constant multiplied with c time plus ln of another constant. So, generally these constants, so I will write is like a and b instead of writing them as constant. So, generally these constants A and B in this case are actually you know determined I mean the same happens also for Yoon-Nelson model and all you will see that there are two or three constants which are present they are actually determined from the existing from you know breakthrough analysis or from an experimental data of the breakthrough that one you know work out or one performs and then it is easier to evaluate all these constants particularly the uncertainty involves in the estimation of the rate constants or the mass transfer which has the effect of the overall mass transfer rate. So, those constant these constants are actually evaluated from fitting the concentration profile with time, up to the breakthrough limit for a specified you know flow rate and this bed height.

And once these constants are determined then the model can be applied for other different flow rates and different bed lengths and that is how this model is useful in designing fixed bed adsorption column. So, I hope all of you you know found this lecture useful and you have understood the different types and the background of the other model models that is present in this case. And hopefully this will be useful in your work to determine and to model fixed paid adsorption column of varying flow rates and varying heights. Thank you. See you everyone in the next lecture.