Course: Adsorption Science and Technology: Fundamentals and Applications

Instructor: Prof Sourav Mondal

Department: Chemical Engineering

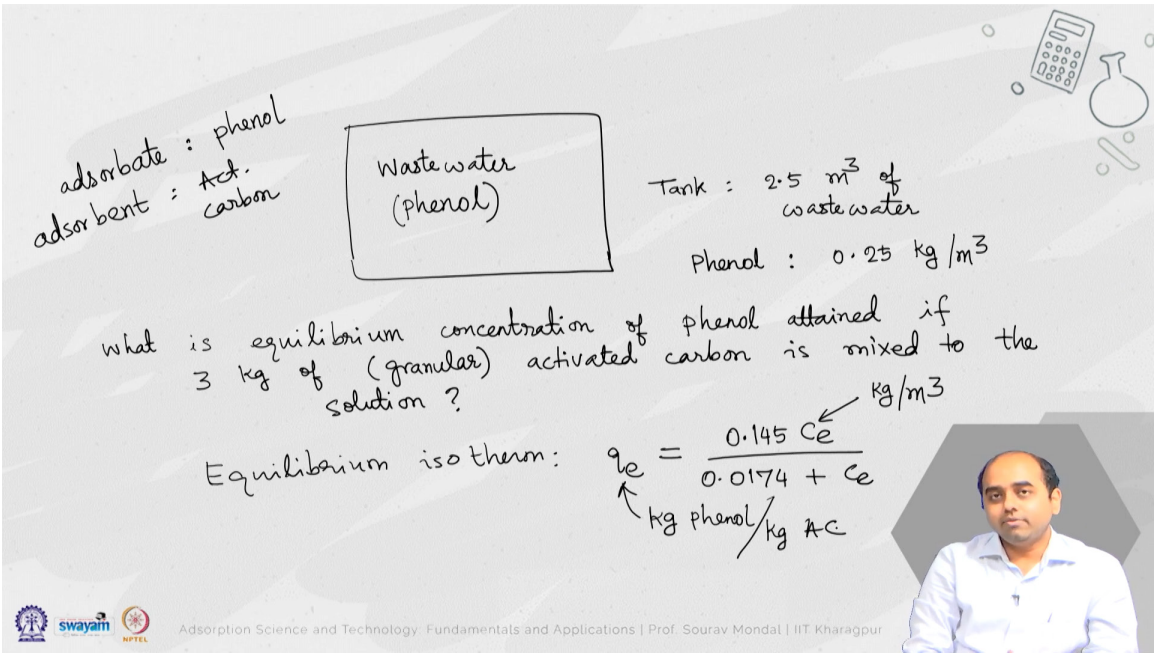
Institute: Indian Institute of Technology Kharagpur

Week 02

Lecture 8 | Equilibrium Modelling – I

Hello everyone. Welcome to this lecture on adsorption science and technology. In this course, as you know, we are talking about different kinds of adsorption processes, principles, isotherms, mechanisms and applications. In this lecture today we are going to talk about the some of the example problems which can be solved or which can be analyzed based on the equilibrium concentration or the equilibrium theory particularly involving Langmuir isotherm at least for this class. So, we will see how you know we can model or we can work out simple scenarios or situations at equilibrium of course using this adsorption principle. So let us say the first scenario that we are going to look into is of you know a treatment process or a separation process.

So let us say we have a waste water solution in a tank. This waste water is present in a tank and this waste water contains primarily the phenol as one of the pollutant which needs to be removed. And this is a very classical you know problem of wastewater treatment particularly at the end stage or in the tertiary treatment system where you want to add we want to remove or treat this final you know wastewater before it can be discharged into the environment, the contaminant needs to be removed and a particularly low concentration of you know this kind of organic chemicals is very dangerous or hazardous for the environment. So, their removal is very necessary and since this concentration of the species is very low adsorption founds to be often very useful and it is a selective process as you know.

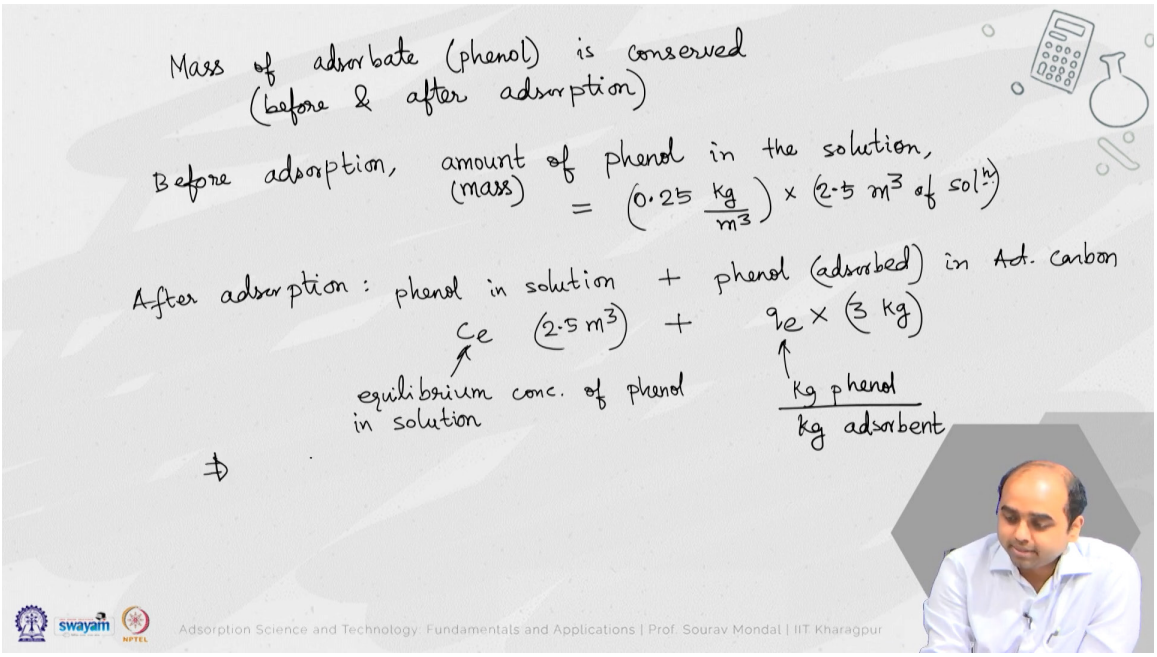


So, let us say the tank volume or the tank contains 2.5 meter cube of the solution of waste water which needs to be treated of course, to remove phenol and the phenol present having a concentration of 0.25 kg per meter cube. This is particularly very high concentration if you know the phenol concentration for environmental discharge should be should be ideally very low and this is generally very harmful for industrial effluents from pharmaceutical companies where the phenol is generally produced in large quantities. Not only pharmaceuticals even fine chemicals, pesticides or agricultural industry these also produce a lot of these phenol or otherwise this phenolic compounds during this process and can contain very high levels of phenol in the waste water that needs to be treated.

Now, the idea is to we have to find you know what is the amount of the adsorbent that is needed to purify or to treat this solution from this system. So, that it reaches or the concentration in the treated solution reaches below a particular permissible value. So, the question stands as what is the equilibrium concentration of phenol attained if let us say 3 kg of activated carbon is mixed to the solution. So, let us try to work out the equilibrium concentration first and then we can solve the inverse problem that to achieve a particular level of the equilibrium concentration what would be the amount of the adsorbent that would be needed in that case in this case. Now, as you understand this is the adsorption follows this equilibrium isotherm.

So, the knowledge of the equilibrium isotherm is very important. So, we can write down

the equilibrium isotherm for this system. So, in this case, please make sure that you realize that the adsorbate is the phenol and the adsorbent is the activated carbon . So, the equilibrium isotherm is the relation of the phenol concentration present in the solution phase and present in the activated carbon. So, this Qe is represented as 0.145 Ce by, So, this is the classical Langmuir isotherm model or the two constant model, the units are very important here. So, in this case the C e is in terms of the units of kg per meter cube because the coefficients are the constants in this isotherm equation follows or is dependent on the on the this units of the Ce and the Qe and the Qe represents the kg of the adsorbate which is the phenol per kg of the activated carbon. So, essentially Qe is a unit less or a dimension less quantity, but it is very important to understand that it is the kg of phenol per kg of the adsorbent that is how the equilibrium concentration in the adsorbent phase is described in this case. Now, the this we do not know I mean from the equilibrium isotherm it is a relation between equilibrium concentration in the solution phase to the equilibrium concentration in the adsorbent phase. So, both of these is unknown in this problem because we do not know what is the equilibrium concentration neither in the solution phase nor in the adsorbent phase.



So, we only know the initial conditions and we only know the total mass of the adsorbent. So, to solve this problem we need to find out or we need to you know take help of the mass conservation of phenol. So, the idea is something like this - that the mass of phenol is conserved, right I mean before and after adsorption. So, before the adsorption whatever the phenol that was present in the solution, after the adsorption this has moved to the solid phase or to the adsorb part of it has moved to the solid and the or the adsorbent phase and part of it is present in the solution phase equivalent to and in the in the form of

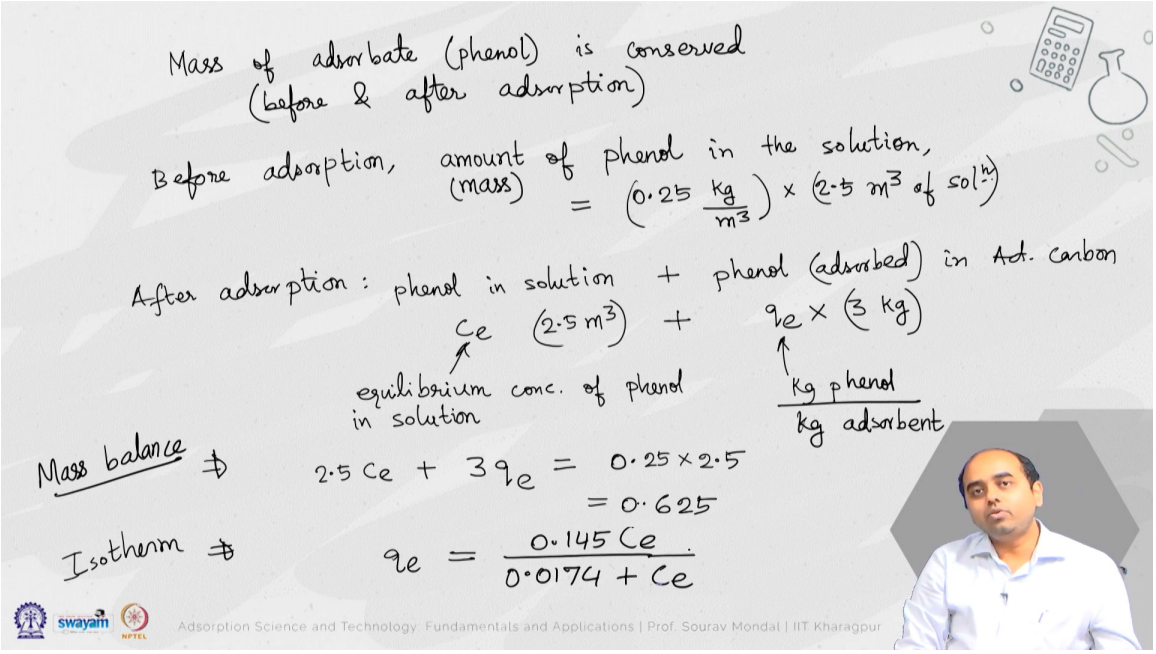
the in the in the solution phase in the liquid. So, this total amount of the phenol is conserved initially and after adsorption.

So, before adsorption if we try to write the total amount of phenol that is present all of it is present in the solution. So we have the concentration of 0.25 kg per meter cube. And if that is multiplied with the total volume that is 2.5 meter cube of solution, this gives us the amount of the phenol that is present or the mass of the kgs of the phenol that is present in the solution. We just multiply with the concentration with the volume. After adsorption, part of it is present in the solution and part of it is present in the adsorbent. So, phenol in solution plus phenol adsorbed in activated carbon. So, the amount of phenol that is present in the solution, the solution volume remains unchanged.

So, that is 2.5 meter cube, but the concentration is unknown. So, it is multiplied with Ce. So, this is the equilibrium concentration. So, after adsorption has reached equilibrium, the concentration in the solution is the equilibrium concentration. So, the equilibrium concentration in solution is represented by the Ce and the amount of phenol that is present in the carbon. So, it is the Qe which is the equilibrium concentration of the phenol per mass. So, Qe is defined as mass. So, this is kg phenol per kg of the adsorbent is defined Qe is defined in this way. So, this has to be multiplied with the amount of the adsorbent and the amount of adsorbent that is added is 3 kgs in this case. So, this is a balance equation.

So, if we try to write this down mathematically this represents 2.5 Ce plus 3 Qe is equal to. So, this is one equation from the mass balance which relates Ce and Qe. The other equation is of course, the so this is from the mass balance of phenol and another one is of course, from the isotherm which is already mentioned that QE is equal to 0.145. So, now in this case there are two mathematical equations two algebraic equations and two unknowns Ce and Qe. So, if you try to work out I mean or try to solve these two equations which is very simple you just substitute the value of Ce or Qe in this second equation and you can find out what would be the values of this. So, on solving solving this two these two equations you can get the value of Ce around 0.1 kg per meter cube. So, this is kg per meter cube for phenol and the value of Qe is 0.12 kg phenol. So, this is the equilibrium concentration of phenol in the adsorbent per kg of kg of the adsorbent. So, the amount of recovery for this system or for this problem stands as. So, the amount that is recovered or the amount that is recovered is the amount of the phenol that is removed from this system. So, the amount of phenol that is removed from the system divided by the amount of phenol originally present, represents the recovery of phenol. Of course, we do not want to recover phenol we want to just separate phenol, but in case this

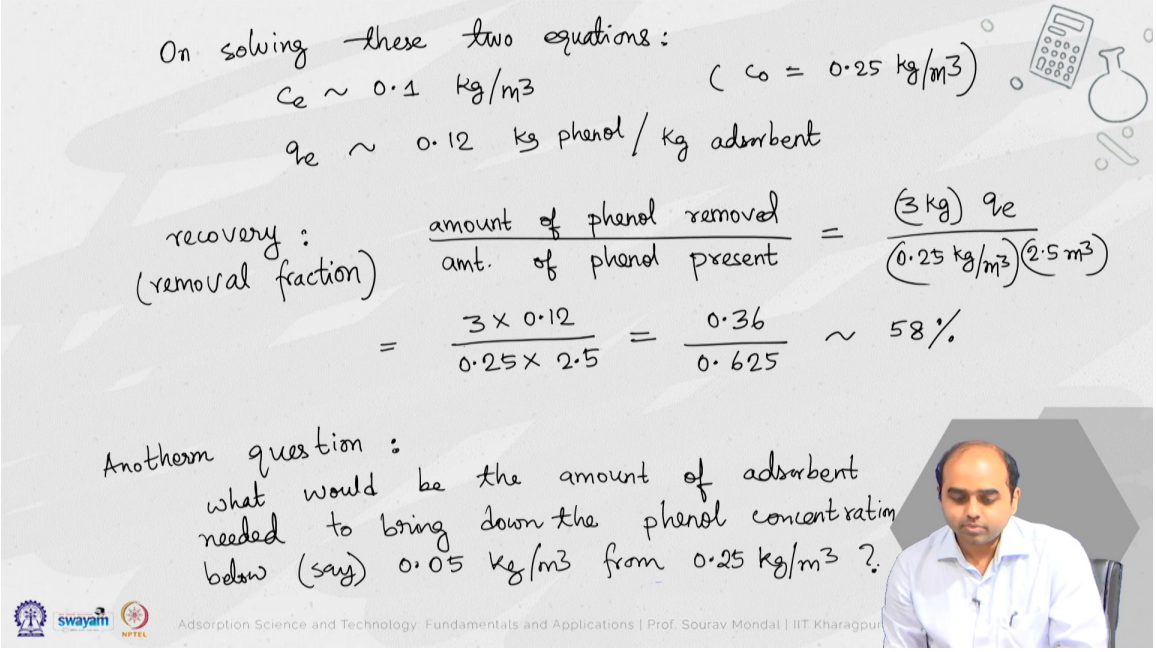
is a value added chemical this is how the recovery of the adsorbate species can be defined.



And in this case the amount of phenol that is removed is 3 times the I mean 3 kg of this adsorbent was that and multiplied with Q e gives the amount of phenol that is removed. And the total amount of phenol that is present we can use the condition before the adsorbent. So, that is 0.25 kg per liter meter cube multiplied with you know this 2.5 meter cube of the solution.

So, this is equal to 3 into 0.12 divided by 0.25 multiplied with 2.5. So, this tends to around 0.36 divided by 0.625. So roughly this stands around 58 percent. So, this represents the amount that is recovered in this case. So, this is what we mean ah by the recovery and at the equilibrium condition. Another you know this variation to the problem stands as like what would be the amount of the adsorbent? So, in this case we have already defined the amount of the you know this, which is present and we are working out what would be the equilibrium concentration and would be the recovery or the removal right. This recovery can also be considered as the removal fraction. But let us say if we want to consider that the equilibrium concentration or the treated solution should be below a particular desired value. So, in this case the final concentration came down to 0.1 kg per meter cube from 0.25. So, originally it was. So, C 0 or the original value was 0.25 kg per meter cube from there it was reduced 2.1 kg per meter cube by addition of 3 kg of activated carbon. So, now, the question is if we want to reduce it to let

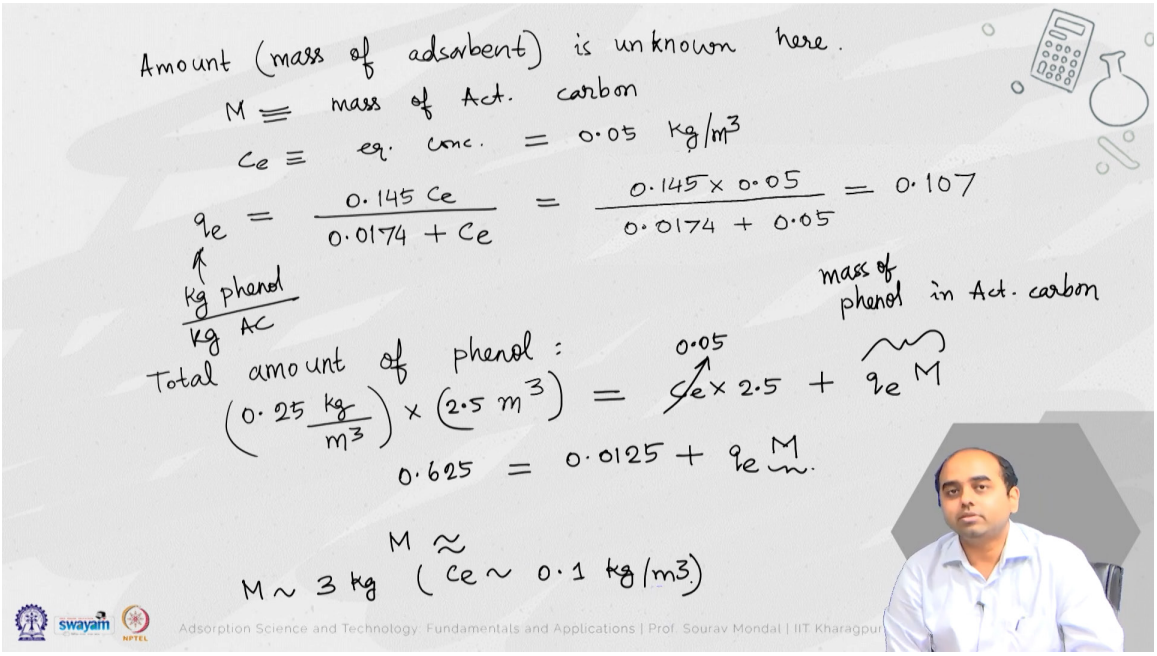
us say to 0.01 levels or 0.05 levels what would be the amount of the adsorbent that would be needed. So, another question on this same topic that can be based on is that what would be the amount of adsorbent needed to bring down the phenol concentration below say 0.05 kg per meter cube from 0.25 kg per meter cube. This is also very relevant because this will help us to determine the amount of material that is needed in this case so that a desired level of the concentration can be achieved in this problem.



So to work so this is a possible variation to this problem which can also be worked out. Let us try to work this out here itself. So in this same problem we see that now the amount of the adsorbent is unknown. So the amount or mass of adsorbent is unknown here. So, let us define the mass of the adsorbent is m. Ce is the equilibrium concentration and in this case the value of the equilibrium concentration is already known from the problem and that is defined as 0.05 kg per meter cube. So, from the isotherm we can work out what would be the value of the adsorbent concentration in the solid phase or in the adsorbent phase. So, in this case if the value of, so this is the you know value of the adsorbate concentration in the adsorbent that is attained at equilibrium because the equilibrium concentration is already predefined in the problem. So, now this is we can work out how much would be the value of Qe and this can tell us that this is the level of the concentration.

So, the value of this quantity tells us that this is the level of concentration that will be achieved in the solid phase or with the activated carbon. So, accordingly we can work out

what would be the amount of the adsorbent that would be needed in this case. So, the total amount of the phenol is once again that we will be using, that conservation equation. So, initially it is 0.25 kg per meter cube this concentration and it is multiplied with 2.5 meter cube, and this is equal to this is equal to ah this amount of the phenol that is present in the solution which is C e into 2.5. Now, Ce in this case is 0.05 plus Qe into m. So, this is the amount of the phenol or the mass of phenol in activated carbon so this comes out to be 0.625 this is and whatever the value of Qe that comes out you can multiply with the value of m so from here the value of m can be worked out in this case and this if you work out the numbers the value of the total mass of the phenol in this case will becoming larger than the value that was used in the previous case which was 3 kg to obtain a concentration of 0.05 or to obtain a value of 0.05 kg per meter cube. In this case, so mass was around 3 kg. And this produced the equilibrium concentration of 0.1 kg per meter cube. In this case, since the equilibrium concentration is lower, the mass of the adsorbent needed for this problem is higher.



So, I hope all of you have understood the principles of this equilibrium calculation. In the next lecture, we will talk about one or two more problems related to this equilibrium based scenarios. Thank you and see you all in the next lecture.