So, this is we will use this in calculations, but this is not a, you can't use it as a property of a chemical. But from this observation what people have looked at is that I can write this 'KA32' as 'wA3' just now we we have also determined the organic carbon content is different. So we will write this as instead of KA32, will write this KA organic carbon divided by, yah, so we will write it even more expendadly.

We will we will say 'm' of A divided by 'm' of OC, 'm' of OC divided by 'm' of 3 divided by, if I break up the numerator into two terms. Here, we are writing this as 'wA3'. 'wA3' is m of A by 'm' of 3 right, if I write that in terms of this. So this first time here is the is the second term here is the content organic carbon containing it's the amount of mass of carbon divided by mass of the solids. So we will give this, we call it as fractional organic carbon and this term here, t hen becomes it's a mass of organic of chemical A over the mass of organic carbon, ok.

This number here becomes a little more normalised. So what it says is if I know what the organic carbon is in general I can now say that the adsorption of a particular chemical partitioning of a particle chemical on organic carbon with reference to water is should be more or less the same. So, I am removing this f OC out of the equations I am separating it out. So I will what I will do is instead I will write 'mOC', 'mA' by 'mOC' into 1 by Rho A2.

This makes it as 'w A OC' by Rho A2 into 'f OC'. If I do this, this number here is a normalised partition constant. So it does not depend on the amount of organic carbon. It depends on the type of organic carbon, ok. You understand, you? Ok. So, here again we discussed in class that there is likely to be variability in organic carbon itself, but then, collection of a lot of data of people have figured out that the organic carbon has a certain range in which it behaves. It's composition does not change a whole lot unless there's exceptional conditions. So people have measured this. So, they have measured this KA32 using experiments like what we have described here. And then they have broken it up. They have also measured the organic carbon and they have normalised it, they have broken, separated the organic carbon content and the ratio of the 'w A OC' by Rho A2 this number this quantity.

'w A OC' by Rho A2 is now called as 'KOC', it's 'KAOC'. 'KAOC2' is our our definition but this is KOC, is a is a generalised term it is used it is there in the Literature as KOC. KOC is the partitioning of a chemical between organic carbon and water with the assumption that organic carbon is a same throughout the entire world which may or may not be true. This is first exercise is that we you have to do. I will ask to go and get organic carbon 'log(KOC)', for, for different chemicals. You will see the range of KOCs, it's not one number. It will vary and it varies for a good reason. It varies for a reason that we just mentioned it it need not be the same everywhere, depending on origin of organic carbon this composition, will change and therefore the number will also change partitioning will also change and it is more complicated than what we give. But this is a convenient methodology to do this. So, KOC is the, is the physical property that can be listed if you assume that organic carbon has a certain property.

So when people measure organic KOC of a new chemical you need a reference right? Where do I get organic carbon from? I have to get it from I can get it from India, I can get from China, I can get it from the US, or Europe, Africa anywhere. Organic carbon which means I get soil from different places and extract the organic carbon and then use it. So, people of standards, so there are standards to which you measure KOC of a particular chemical, you have to use those standard matrices.

So once we have mentioned in the last class called the humic acid and Folic acid and all that, so we use one of those. So, there are standards available in the in the market that you can buy and you can report KOCs based on that. So when you look at the experiment data experimental data for KOC people will mention what is the organic carbon that they have used. They have used one type of ah OC or naturally occurring OC or synthetic compound which mimics organic carbon all these are possible, ok.

So, this log and usually represented as log KOC, because KOC is a big number and you can imagine even if I have a few milligrams of organic carbon, solubilitys of a lot of these chemicals is small, but they have organic they have, they like they like organic phase. So, they all will go there and they will stick there. That's the reason why we use them as adsorbent because their KOC is very big. Partitioning from water to the solid is very high.

That's the reason we use it as adsorption for and that is why soil is considered to be a naturally purifying medium because while, before it goes to ground water it has to go through all the layers in which there are there is organic carbon that will remove, adsorb a lot of these chemicals and so the number is big. So instead of writing 10000 and 20000 all that they'll just convert into log of KOC. So, again the KOC has units, it's the same unit as that.

So, the nomenclature, the convention is KOC is usually in litres per kilogram. KOC has unit of litres per kilogram because it is it is coming from milligrams per kilogram and milligrams per litre. This is the concentration units of any chemical on solid and this is the concentration unit of chemical in water. So this is usually there, so therefore we cancel, sorry if we cancel these two you get litre per kilogram. So that is general, this is convention.

When you see only log KOC, if you say log KOC of of 4 which means KOC is 10 raise to 4 litres per kilogram unless otherwise specified normally. Sometimes people will just give you the KOC and different units. So, 10 raise to 4 litres per kilogram is 10 metre cube per kilogram. They will give you 10 meter per kilogram and that's also valid. But if they if they mention of only Log KOC then it is assumed that units of KOC are litres per kilogram.

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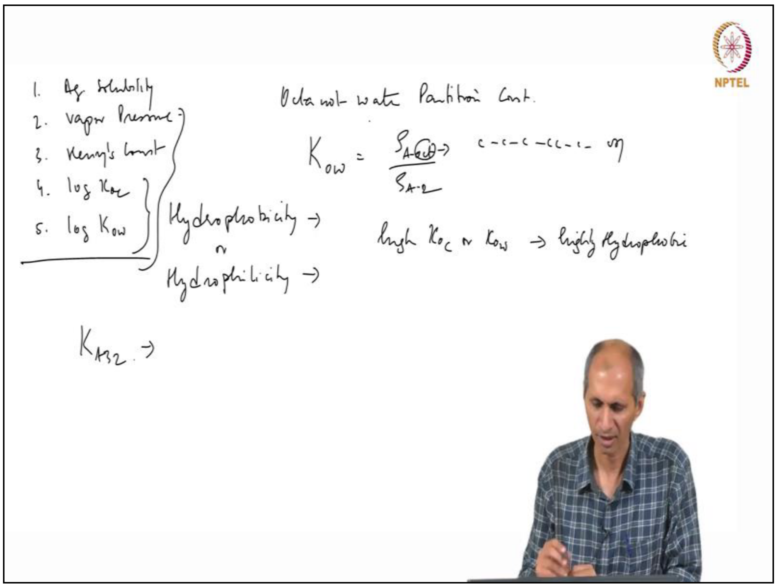

So, in association with log KOC, so we have now properties of we have aqueous solubility, we have vapour pressure, we have Henry's constant, we have log KOC. So in association with log of KOC, log KOC generally gives you the affinity the tendency of a chemical to bind to an organic phase. This is a general assumption, yeah. There is a larger implication of this, so before environmental scientist came about and invented log KOC because it pertains to soil and sediments and all that .

In Pharmacology, in toxicology people look at this number differently, ok. What they look at is if you are eating a medicine or a poison or how toxic a particular material is when you different through different routes, inhalation or oral route. They look at the binding of this particular chemical, its accumulation in the human body in in your tissue and this they call as 'Bioaccumulation'.

This is bioaccumulation also results is is determined by, by looking at the theory there is that most of the blood and all that all the food goes in it gets digested it is going in more or less aqueous solution and it is partitioning between different portions of the tissue, ok, as it is going. So, if a chemical has a very high partitioning between water, water base, aqueous base system and very high organic lipid tissue is considered to be a lipid based this thing, fats and tissue and all that.

So, people look at that partitioning. And so they can have different numbers. They can have KA some bio, some tissue and water. They can do it at different levels. They can take say take some animals they just dump the animals into water put a chemical and after defined time they will see how much of chemical is gone into the, into the animal into, into a fish or something else. That is one bulk thing you can look.

Or you can take a particular tissue you can probe which part of the tissue how much accumulation happening on the tissue itself. So, this bioaccumulation factor is also base it's just like the log KOC. It is the ratio of two concentrations. So in this context people have what is called as KOW. Now this is a normalised number instead of using lipids, they use Octanol. Octanol is used as a surrogate for lipids. ok

So, it is an octanol water partition constant, ok. So this is KOW equals now you will just write it as Rho A Octanol versus Rho A water. This is how it's been determined originally. So they don't use W, they use Rho for some reason. Octanol is a liquid when you are doing the test outside. But in the human body, in the body, tissue is solid, ok. So measurement of that is very difficult. So what people have done is they need a common basis to which in, in which they can estimate accumulation factor.

So KOW or Octanol-water constant. Octanol is considered to be a good surrogate of the lipids so which means it's it's reasonably long Chain and then it has OH group 8 carbons. OH group it looks like the organic carbon. Organic carbon is a long chain hydrocarbon with polar groups at t ends. So, Octanol is not that long but some some numbers so they have chosen it by some on some basis based on analysis of lipids and how they.

So, it is not the actual number that will be there in the human body, but it is notional, it gives you a scaling, it gives you some kind of comparison of of what? What does it give you? If you if you look at log KOC and log KOW both of them will give you a quick idea if you compare the log KOC and KOW they have different Chemicals, organic chemicals. It very quickly looking at the values you can tell whether this chemical will bind to an organic phase or will stay more in the water, whether it likes the oil, likes the organic carbon or like the water.

So this, we come up with another term called Hydrophobicity or Hydrophilicity. Hydrophobicity means it doesn't like water. Now Hydrophilicity means it does not like the carbon, ok. SO, if this is a scale of hydrophobic behaviour. If a chemical is hydrophobic which means high KOC or KOW which means highly hydrophobic. For relative things, there is no absolute terms hydrophobicity. There is no absolute, there is relative one chemical versus another chemical.

One of them will or you can that chemical which has log KOC or KOW of 1 versus log KOC or KOW of 4 which means this is 1000 times more than that. So, this one will accumulate 1000 times more than that. So, they will do this on the basis of, it also gives you some idea of how much hydrophobicity can be enough if you want to design a particular chemical especially for this is used a lot in Pharmacology.

As we discussed Pharmacology looks at how much of accumulation in the body is medicine.
You need the medicine to bind to a particular site in order to work. So chemical is not at all hydrophobic and it's hydrophilic then it will not accumulate anywhere. It will go out or it will pass out body will send it out without any adsorption or any accumulation. So there are various applications to this, both environmental as well as this thing.

But the property of KOC and KOW is used as an index to see whether just quickly, quick reference. You can look at all these properties and say where the chemical is going to be. If I look at all these properties, and I can quickly give a qualitative view of you know this chemical is likely to be more in air than in water or it will not be water in the sediment soil it will come out very slowly. Which means you can make very quick decision as to where your attention should be, your focus should be, on, on remediation or treatment or whatever that you need to do subsequent decision to it.

So these are all these are important properties and most of the chemical structure are concern to us these properties are listed. So, these last 2 pretty much except the last four most of them is organic chemicals is the focus. The first one you have both organic and inorganic. The partition constant KA 32 we are worried about it from both inorganic and organic. Both of them will partition, but the KOC theory only applies to organic Chemicals. It does not apply to inorganic chemicals.

So we will talk about inorganic chemical tomorrow. What happens to them and how how does KA32 changes for that? But you cannot generalise it like this. You still have to, you have to find out you have to find out other set of conditions which is not very easy you have to do it very site specific and there is no generalised theory based on for that.