

**Life Cycle Assessment**  
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**Lecture – 28**  
**Chemical Release in Environment**

Welcome back. As you know we are on in the week 6 of this course. So, we have already covered 5 weeks this is this would be the third module of week 6. So, hope that you are enjoying this course. So, far, let us say if you remember for the previous module and previous week we had gone through the details of how life cycle analysis is performed also give you an example later on in the week 8 we will look at some more examples and we will also have some example problem solving which will be include which will be uploaded as a separate video later on.

So, today we will for this particular module will try to look at when we say this lifecycle analysis. If you remember, we were looking at the different chemicals how the chemicals are what is the environmental footprint, but if you think of a realistic environmental problem where you have release of chemicals. So, you ultimately why we are worried about all these. So, we are worried about environmental impact from human activities including we manufacturing and usage of lot of anthropogenic chemicals.

So, when we say anthropogenic chemicals they are manmade chemicals they are not natural chemicals for the anything which is made naturally by mother earth mother earth had a mechanism to take care of that particular material that is made, but when we make lots and lots of material in our factories and dump it on mother earth when I say mother earth I am essentially talking about water soil and potentially to air we have to understand what how this chemicals are going to behave in different medium and that kind of dictates how what kind of risk it may have. So, today we will look at some of the basics of that.

So, topic for today is environmental release of chemicals and its fate and transport.

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## Environmental releases

- A material, at the end of its useful life cycle or as a consequence of its production or use, is released into the environment
- Will its release pose significant environmental or human health risks?
- Will the chemical degrade in the environment or will it persist?

So, what is how the materials gets released material usually when say- we in the lifecycle if you remember if we were talking about from the raw material acquisition all way to dispose of; so at the end of its useful lifecycle or even during the production phase. So, when you are when you are doing some mining activities. So, when you do the mining activities as part of the bio product you produce mining over burden you use lot of say for example, in the frocking industry they use lot of water and most of that water when it comes out it is highly contaminated water. So, those water needs to be treated as well. So, the material at the end of its lifecycle either as a consequence of production or use when the chemicals associated with that particular material gets released into the environment.


So, the question is will it release will they release post significant environmental or human health risk because if you remember what to those impact categories we had the impact categories that we chose for the lifecycle impact assessment when we say this impact assessment how those how it decides whether there is a significant risk or there is no risk. So, for that this fate and transport basics needs to be understood and at the same time whether this chemical will exist as it is or whether they will degrade to newer chemicals they will make the daughter products and once it degrades or even if it is stay stays as it is how long it will stay as it is how persistent is that particular compound. So, environmental release it can happen when the things towards when did the any product or material is disposed off or during the production phase the waste that is produced.

So, the question again there are kind of question will be what is the significant and environmental human health risk for that particular material and whether the chemical will degrade in the environment or will it persist. So, as I said what will happen to it over time?

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**Table 4-4 Chemical Properties Needed to Perform Environmental Risk Screenings**

Environmental Process	Relevant Properties
Dispersion and fate	Volatility, density, melting point, water solubility, effectiveness of wastewater treatment
Persistence in the environment	Atmospheric oxidation rate, aqueous hydrolysis rate, photolysis rate, rate of microbial degradation, and adsorption
Uptake by organisms	Volatility, lipophilicity, molecular size, degradation rate in organism
Human uptake	Transport across dermal layers, transport rates across lung membrane, degradation rates within the human body
Toxicity and other health effects	Dose-response relationships



So, there are different environmental processes as you can see in this particular table which is taken from the book that I suggested you to kind of what are the ref I am not say not required, but one of the suggested text book which is the part of the course description this you can this is this is a particular table comes exactly as a table of four point four from that particular book. So, there are when whenever we look at the environmental risk screening we look at several environmental processes as you can see over here we have dispersion and fate dispersion and fate is whether the how easily the material will get dispersed into the environment especially it is very much related to when we talk about the air pollution problem how things will get dispersed and what would be its fate and some of the some of the properties which is relevant to that is volatility means volatile is the material.

So, say as you open you open a bottle containing some organic acid or something if you can smell it what does it mean it means that that material if that chemicals inside the bottle I part of it went into the air phase otherwise you will not be able to smell is not it anything you can smell through your nose is only possible if things are there in the air

phase around us otherwise if it does not come in air phase will not be able to smell it. So, and whether things will come to air phase or not depends upon whether the material is volatile or it is not a volatile substance.

So, volatility is very important in terms of dispersion as well as the fate density of the material why density is important anything which is lighter than air will have a tendency to go much higher and can go with the wind on a long distance anything which is heavier than air will have a tendency to stay at the bottom if you remember if you pretty much sure that you must have heard about Bhopal gas tragedy, but Bhopal gas tragedy if you if you know that the gas which was involved was methyl isocyanide. So, methyl isocyanide is heavier than air. So, that is why we in from the myth from the Bhopal gas tragedy we had a localized impact, but much severe impact the impact was in an around Bhopal city, but not too much away from there because it is heavy it could not travel too much, but then it has a severe impact because the concentration was pretty high it did not get mixed with the air very well had it been lighter than air it could have gone up.

So that the impact would have been less, but and at the same time the with the air mixing it could have got diluted, but and that is on the positive side on the negative side effects lighter than air things may travel along a distance, if because it will travel with air. So, that is, but since it get diluted for most of the most of the situation you will have less impact as opposed having a something heavier than air.

So, density may it is that density is very important for that part melting point whether things will become a liquid or be remain in solid we know that water solubility how much it will be soluble in water something which is easily soluble and water can be carried by water if it is not soluble it will just stain the it will just stain the solid phase then whether our waste water treatment plant can remove it or the effectiveness of waste water treatment plan see most of the waste water treatment plant we have in the world today they are designed to treat for organics. So, since we have higher organics coming from fecal matter. So, they are essentially a set of aerobic and anaerobic system where we are focusing on removal of BOD biological oxygen demand which is essentially coming from organic load and ammonia.

So, we have nitrification de-nitrification and all those things are happening some are doing phosphorus removal nutrient removal and all that, but if you look at the chemicals the way the chemicals are being produced today most of the waste water treatment plant is not designed to treat for those chemicals many many of this emerging contaminants we are taking lots of medicines we are taking lots of pharmaceuticals we are taking those pharmaceutical products we say you take 100 m g tablet your body only observes may be 10 m g, 20 m g, 30 m g and rest of it goes out as part of your urine or the fecal matter mostly urine when it is goes in the waste water treatment plant the waste water treatment plant is not designed to treat all these emerging contaminate not designed to treat for this pharmaceutical products.

So, and then they end up in the water bodies in the surface water bodies. So, that is the effectiveness of the waste water treatment is essential in terms is to know what will happen to it if the waste water treatment plant can treated then mostly it will be in the sludge and because as I have told you earlier as well in many probably in several videos that we cannot destroy anything which is on the periodic table. So, we can only change its form. So, if it is if it is not in the water phase if it is not in the treated water affluent it will be in the biosolid, but then that is a different kind of problem bio solids means you can manage it much easier if it gets into the water the managements becomes little bit more tricky.

So, that is in terms of the dispersion and fate there are the relevant properties many of these properties as you can see are repetitive because they have they do impact persistent in the environment that is a second environmental process that will depend on how easily it can be degraded what is the atmospheric oxidation rate if it gets hydrolyzed what is the acqua hydrolysis rate. So, all those your chemical kinetics that is that will essentially like what is the rate of reaction and for that.

Remember we use the term you must have heard in your high school or a may be in first year or engineering or science courses as well we call it a term half life half life as you know half life for any product means at what time say you start with x amount of that material if the concentration is x milligram per liter or x milligram per kilogram by what time it will become half of x. So, x divided by 2. So, that is the half life. So, sorted the half life be higher is the degradability higher the half life it is; that means, our chemical is more persistent. So, that is those are those kinds of rates have been given here rate of

microbial degradation and absorption. So, all these things are related to the rate. So, that is your chemical kinetics part.

Then uptake the organism whether organisms will be up we are able to uptake it volatility if it is higher volatility things go to the air phase organisms may not be able to uptake it lipophilicity what is again this is a newer term now we have seen it in the other 2 lipophilicity is basically affinity for lipids remember it is similar to remember we if there is a term hydrophobicity and hydrophilicity hydrophobic means phobia means fear is not it we the many times you say phobia of this phobia of that. So, hydro excuse me hydrophobic means something which is fearful of water if anything is fearful of water it will not dissolve in water very simple just think in a logical way anything which does not like water will probably does not dissolve in water, it will like to remain in the solid phase hydrophilicity means affinity for water they love water affilicity means they love water.

So, if they love water they will get into the water and they will dissolve and then it becomes in a dissolved phase similarly lipophilicity means they have a tendency to this to react with lipids and if higher the lipophilicity; that means, that more will be the uptake by the organisms because in our body we have like lipids and all those things and. So, this molecules or chemical the; if it is lipophilic it has affinity with our like the lipids in our body it will get absorbed on lipids and then you it will build up in our body. So, that is important.

Molecular size that is the another one molecular size is very very important in terms of how the trap part will travel or the things can be up taken bigger see when you when you hear about air pollution problem in Delhi luckily this year this winter we did not had that much of an issue, but every winter we get an issue of high air pollution problem in Delhi during the winter months in one term you hear a lot when we talk about air pollution issues is particulate matter  $PM_{10}$ ,  $PM_{2.5}$  means any particle less than 10 micron  $PM_{2.5}$  means particle less than or equal to 2.5 microns.

So, molecular size the size of the particle is important is smaller the size of the particle they can easily get into the body. So, it is like a it will go into our nose our nose system we if you insider one inside as you can feel it there is a small small hair inside the nose and that hair has a purpose those is small hairs are there they acts as a filters they have

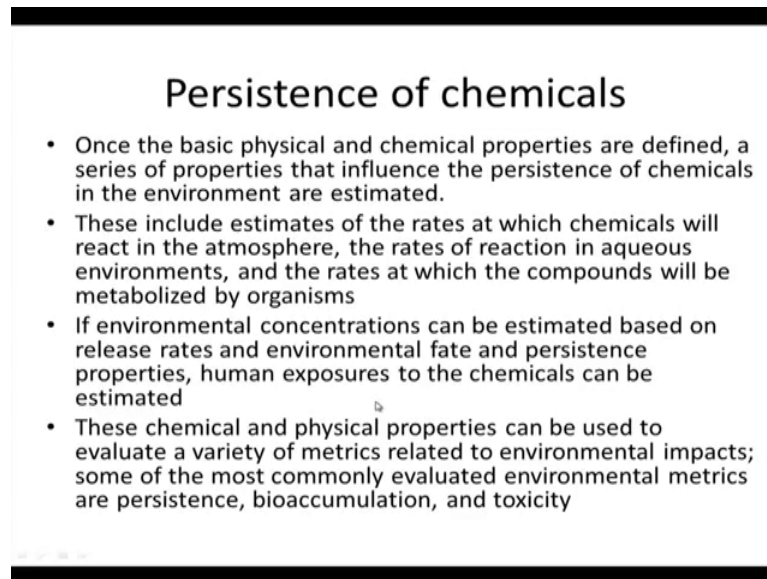
any anything when we inhale things any contaminant which is which can be throat which can be trapped by this filter in our nose it does that so, but smaller the particle our nose will not be effective.

So, that is why p m 2.5 is much dangerous and p m 10 and p m 10 is dangerous and anything bigger than that. So, a smaller the particle it can easily go through our nose and then it can go to our lungs. So, that is becomes a problem molecular size is dictates how the uptake could be the organism degradation weight in organism like how the things will degrade within the organisms as well that is also important then human uptake whether it will go through our dermal layers what is dermal layers it is our skin.

So, whether say if I am touching something which is this is my hand has some chemicals and then I put this hand on top of it now whether this were some of this chemicals will go through here this hand had some had a gloves I did not had any gloves on this one by mistake I put the hand on the gloves and some of the chemicals from the gloves can get in to my skin and get into the body that is the dermal contact that is the dermal layer then the what would be the transport across the lung membrane with how it will go with these the lungs we talked about that for the air pollution degradation rates with the human body or it will degrade within our human body.

So, all these factors needs to go in terms of the environmental risk screening and then you look at the toxicity in the other health effect that gives you the those response relationship and nothing we talked about that earlier.

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**Persistence of chemicals**

- Once the basic physical and chemical properties are defined, a series of properties that influence the persistence of chemicals in the environment are estimated.
- These include estimates of the rates at which chemicals will react in the atmosphere, the rates of reaction in aqueous environments, and the rates at which the compounds will be metabolized by organisms
- If environmental concentrations can be estimated based on release rates and environmental fate and persistence properties, human exposures to the chemicals can be estimated
- These chemical and physical properties can be used to evaluate a variety of metrics related to environmental impacts; some of the most commonly evaluated environmental metrics are persistence, bioaccumulation, and toxicity

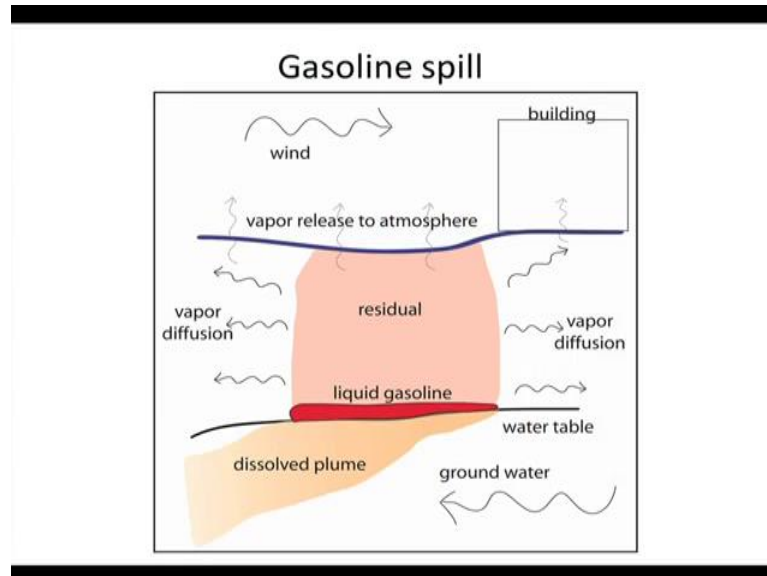
So, in terms of the persistence of the chemical once the basic physical and chemical properties are defined we can look at a series of again these do not do not worry too much about this slides has lot of text in there this was given to you just to kind of help you for reading purposes. So, that you can it is like a summary of the book chapter that rather than which can help you at least I want you to at least read this I will encourage you to read the book chapter as well, but that is why some of these like a small small paragraph bullets which is not very common this particular chapter and some other module you will see that I usually I do not like this we have slides, but just to give you some more information and as you know will provide you the PDF file of the slide as well.

So, this kind add a reading material for you so, but the basic concept just if you; if for the lecture part you can always read it later, but for the lecture part the basic concept here is the physical and chemical properties of any chemical will define whether it is persistent and whether it will get broken down how quickly it will broken down then we talked about the rate we have to estimate the rate will tell us how long it will take in terms of half life whether it goes whether it when it is reacting with the aqueous environment how what is the rate of reaction how quickly they produce and like a newer product and the environmental concentrations can be protected can be estimated based on the rate of reaction based on what happens in terms of the environmental fate human exposure can be calculated along that way.



So, they can we can come up with this chemical and physical properties they can be used to evaluate a variety of matrix we can come up with for its environmental impact and all that. So, that is kind of in nutshell how we look at the in terms of the environmental release it whether it chemical is persistent how it will degrade and different aspects associated with that.

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So, now let us look at a scenario like a like a practical scenario which can potentially happen. So, here and thus it do keep happening from time to time. So, if you have a say you are driving on a highway and see they are on side of the road there was a truck tipped over in the previous night due to some problem of the other the truck as it truck tipped over and then we have a release of gasoline into coming into the system. So, as you can see if it is here that is the top line this is this kind of shows you the surface layer. So, it is of the side you can assume it is as a side of the road the truck has stilled over. So, that and there is some release of liquid gasoline; gasoline is a petrol and then you have this plume that you see here light sorry light this peach colour that is show plume where this gasoline has travelled down and then it goes and this is our the lower black line is that water table. So, gasoline is sitting on top of the grid water table gasoline does not dissolve in water very quickly.

So, it takes time to dissolve, but it does dissolve part of it does dissolve and then you see a plume of the dissolve plume going in between we can have some vapor diffusion going

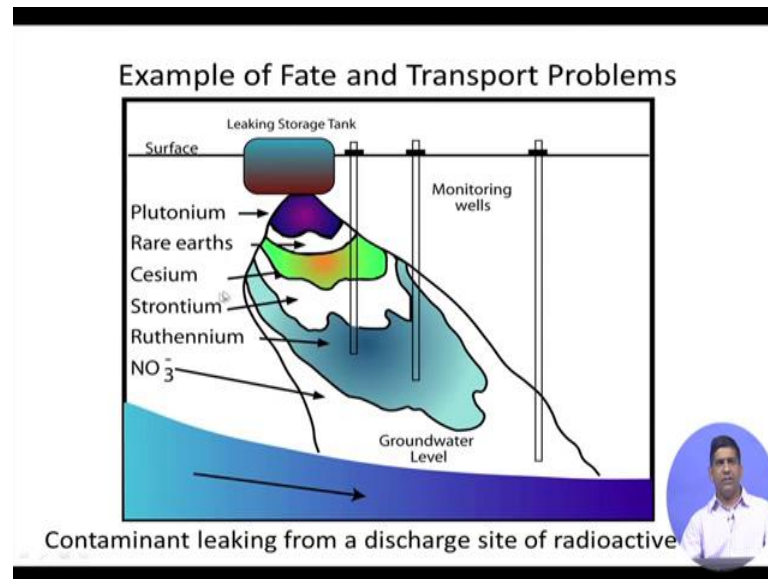
around between the soil this layer between this point and this point is called Vadose zone or unsaturated soil layer. So, there are in the; we have some pore spaces this pore spaces have some air pockets. So, this vapor which is been diffused can take replace some of those air pockets and take those positions once you go below the ground water table you are essentially all those things those pore spaces are filled with water because that is the saturated zone.

So, you do not have you cannot have things diffusing in terms of a in terms of the air part, but you can have the liquid dissolving which you see over here dissolved plume which is happening and what the plume is going in this direction just because it very simple answer because ground water is in that direction at the ground water be on this on the right hand side the plume would have gone on the right hand side as well because the ground water will carry these chemicals with it and that is called advection that is the phenomenon of advection. So, where the contaminant is carried by the media and we as the media flows through.

So, that is your say we you had some chemicals in their gasoline as you know is not one chemical it is a mixture of several chemicals. So, B tex is a very prominent of them B tex is benzene toluene ethylene and xylene. So, they all have different physical chemical properties. So, there will be some vapor diffusion there will be some vapor to that then we have if you have a building and then this is the basement of the building or like the base of the building and if there are some cracks some of these vapors can make into those buildings as well. So, once the vapor gets released into the atmosphere the wind can carry it to a on a longer distance too although it would be diluted ford.

So, this is a this gives a scenario this is also known as the conceptual diagram many times you get the concept that is a conceptual diagram etcetera or concept where it is a conceptual diagram in terms of how the this the any release of chemical what are the different things that will happen into the environment in the near (Refer Time: 21:07) of that particular spill. So, that was one example.

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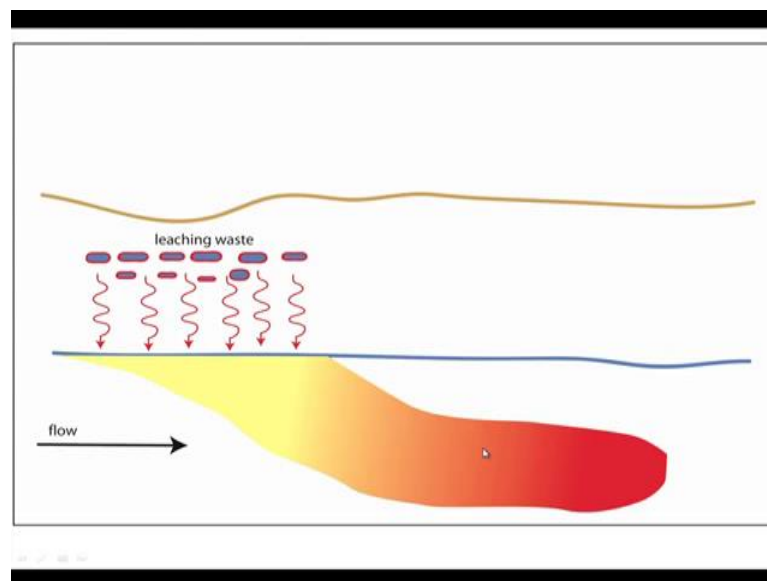


Now, the other example let us see if you have a leaking storage tank that is a very common say if you were leaking a storage tank of a radioactive waste. So, there are different contaminant that can potentially leach off now you see a these different colored graphs these are called plume the as you saw in the previous example as well previous slide as well there was a plume similarly here we have a plume and for different types of chemicals coming out from these leaking storage tank of a radioactive waste we have plutonium we have rare earths we have cesium, strontium, ruthenium, ruthenium and also nitrate. So, based on their physical chemical reaction with the soil layer with the view by the media; which are there on this side like the based on their interaction with this different the soil media we see that different chemicals from this radioactive storage tank radioactive waste storage tank just traveled differently.

So, we had a we had a travel of different if you like plutonium had traveled very less, then the rare earth then the cesium then the strontium ruthenium and the nitrate nitrate is actually easily dissolved in water. So, it can travel with water much quicker with any soil water which is present and, but this other elements which was there in radioactive waste the reaction based on the reaction with the soil media the things will behave differently and then as you can see in the figure we had the monitoring wells. So, how will decide how we draw these plumes as illustrated in the figure as you can see that we have different plumes boundary has been defined and this these are based on these kind of monitoring wells.

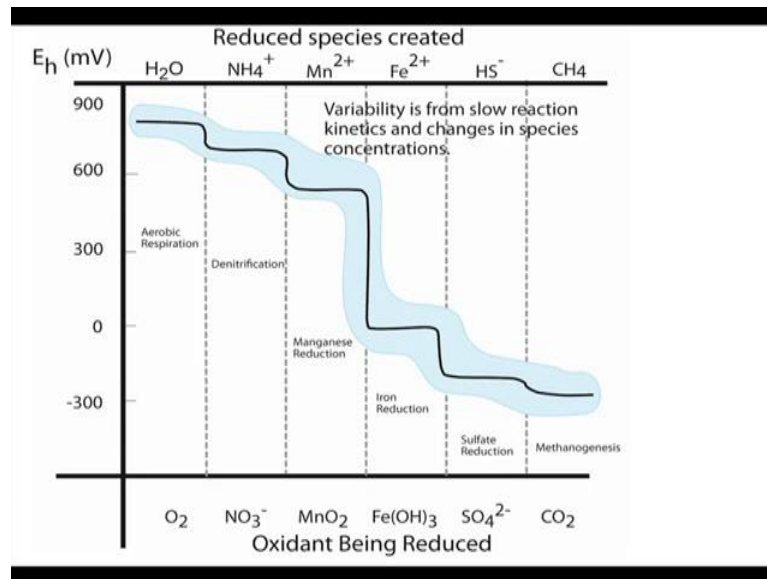
So, you have to do a series of monitoring wells across this contaminated site to give you an idea of how far the waste has traveled how far the different chemicals have traveled. So, that is and it we can we can model we after we get some of these data we can also model and to say try to find out that how long it will take for some of these contaminant to travel all the way to the ground water level. So, after we collect some basic information data from our experiments we can do this we can do that exercise.

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Another example say if you have a landfill kind of condition you have a leaching waste is leaching off because of the different chemical leaching then you have a ground water flow in this direction and you see a kind of a plume building up and again the different chemicals will be there, but they based on the affinity for the soil affinity for all the things that is happening there and their interaction with different media with this they have they are with a plume will have kind of different stretch for different kind of chemicals.

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In the natural environment there are when we when we talk about any of these organic especially organic chemicals or organic matter when they get released into the environment one of the thing is they have to degrade organic matter degradation essentially means that you are things are moving into things are organic matter gets oxidized. So, when they are oxidized something has to get reduced. So, when things have to get reduced there has to be have a electron acceptor remember from your I will I will not go in detail on that just to re you revise that part of a chemistry if you do not remember that.

So, once there is a any reaction we have a one in the oxidant as well as area oxidation and reduction happens in the same time for oxidation there will be an like a release of electron and in reduction electron is accepted. So, if you look at this sketch again. So, first you will see there are reduced species are created based on in the aerobic respiration we have the water which is the reduced species denitrification you have ammonia and ammonium ion then you have manganese reduction iron reduction and sulfate reduction, and then finally methanogenesis where reproduce methane gas. So, those are and these are the oxidants being reduced.

Here we have oxygen then nitrate then manganese oxide then iron oxide then sulfate then CO<sub>2</sub>. So, these are what it is getting reduced and based on this like a based on the e h e h

of the EH means the Redox potential of the system we know which one will be preferable SY for reduction.

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Property	Definition	Significance in Estimating Environmental Fate and Risks
Melting point ( $T_m$ )	Temperature at which solid and liquid coexist at equilibrium	Sometimes used as a correlating parameter in estimating other properties for compounds that are solids at ambient or near-ambient conditions
Boiling point ( $T_b$ )	Temperature at which the vapor pressure of a compound equals atmospheric pressure; normal boiling points (temperatures at which pressure equals one atmosphere) will be used in this text	Characterizes the partitioning between gas and liquid phases; frequently used as a correlating variable in estimating other properties
Vapor pressure ( $P_{vp}$ )	Partial pressure exerted by a vapor when the vapor is in equilibrium with its liquid	Characterizes the partitioning between gas and liquid phases

And that that they finds how the waste will behave in a natural setting in terms of it is reduction going on other then again this couple of slides more where we have a kind of given a very basic definition of what is melting point what is boiling point what is vapor pressure and you all know about all that this is just to give you a recap of what they are because you know the melting point is temperature at solid and liquid coexist boiling point is when it goes from the liquid phase to vapor phase partial vapor pressure is the partial pressure exerted by the vapor when the vapor is a equilibrium with the liquid. So, those are; was there and that we how we use a those information are also provided just for your benefits.

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Property	Definition	Significance in Estimating Environmental Fate and Risks
Henry's law constant (H)	Equilibrium ratio of the concentration of a compound in the gas phase to the concentration of the compound in a dilute aqueous solution (sometimes reported as atm-m <sup>3</sup> /mol; the dimensionless form will be used in this text); $C_A = H C_W$	Characterizes the equilibrium partitioning between gas and aqueous phases
Octanol-water partition coefficient (K <sub>OW</sub> )	Equilibrium ratio of the concentration of a compound in octanol to the concentration of the compound in water; $C_O = K_{OW} C_W$	Characterizes the partitioning between hydrophilic and hydrophobic phases in the environment and the human body; frequently used as a correlating variable in estimating other properties
Water solubility (S)	Equilibrium solubility in mol/L	Characterizes the partitioning between hydrophilic and hydrophobic phases in environment

Some others Henry's law constant Octanol water partition water solubility. So, these things need to be kind of revised if you have not if you have forgotten about it.

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Property	Definition	Significance in Estimating Environmental Fate and Risks
Soil sorption coefficient (K <sub>OC</sub> )	Equilibrium ratio of the mass of a compound adsorbed per unit weight of organic carbon in soil (in µg/g organic carbon) to the concentration of the compound in the water phase (in µg/ml); $C_S = K_{OC} C_W$	Characterizes the partitioning between solid and liquid phases in soil which in turn determines mobility in soils; frequently estimated based on the octanol-water partition coefficient, and water solubility
Bioconcentration factor (BCF)	Ratio of a chemical's concentration in the tissue of an aquatic organism (C <sub>AO</sub> ) to its concentration in water (reported as L/kg); $C_{AO} = BCF C_W$	Characterizes the magnification of concentrations through the food chain

A same thing with the soil sorption coefficient or the bio concentration factor soil sorption coefficient is the equilibrium ratio of mass of compound is of per unit of weight of organic carbon in the soil. So, that is kind of gives you a how good the absorption will be in case of any in case of any chemicals passing through certain soil layer. So, it can

you can do the partitioning of solids and liquid phase in all that kind of stuff bio concentration is basically see how the things concentrate along the (Refer Time: 27:40).

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### Using property estimates to evaluate environmental partitioning, persistence, and measures of exposure

- The problems associated with estimating environmental exposures are complex
- Consider the relatively simple example of calculating exposure through drinking contaminated surface water
- Assume that a chemical is released to a river upstream of the intake to a public drinking water treatment plant

So, all these probably we have already kind of know about that. So, we try to based on with the like that we have to essentially do some estimation and in terms of environmental partitioning persistent and measure of exposure. So, that we take many as we know the environmental exposures are complex so, but if the chemical is released in a reverse stream of like of the (Refer Time: 28:05) or the system so that will be take you water contamination is will be a problem.



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**To evaluate the exposure we would need to determine:**

- What fraction of the chemical was adsorbed by river sediments
- What fraction of the chemical was volatilized to the atmosphere
- What fraction of the chemical was taken up by living organisms
- What fraction of the chemical was biodegraded or was lost through other reactions
- What fraction of the chemical was removed by the treatment processes in the public water system

So, the question that we need to ask about that is what fraction of the chemicals was absorbed by sediments what fraction of the chemicals was volatilized what fraction of chemical was taken up by living organism what fraction of the chemical was biodegraded or be lost what fraction of the chemicals was removed from the treatment process all these questions needs to be answered when we are trying to do this environmental like a characterization and risk so kind of some of in summary of kind of summarize this with this last slide on this particular module.

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**Direct Use of Properties to Categorize the Environmental Risks of Chemicals**

- Chemical and physical properties can be used to estimate environmental footprints
- Another approach is to use the values of properties to directly categorize the environmental risks of chemicals and to classify the persistence and bioaccumulation of chemicals

So, we \ have to get the information about the different properties and that helps us to characterize the environmental risk chemical and physical properties as you as I listed few of them as well they can be used to estimate environmental foot print and which is again we have those all these information kind of already goes into this LCI when I say that you can use certain database you can use certain impact assessment methods. So, all these information is already built in those tools that is why it is important for you to understand what goes on behind the software; software does it things for you, but if you have to tweak that software if you have to use it for your own kind of set of criteria you should be able to tweak the software and then that case you need to understand some of the basics.

So, chemical and physical properties are important which we talked about another approach is to use the values of property directly to characterize the environmental risk and then we classify it whether it is a persistent bio accumulation bio accumulation potential and all that.

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<b>Table 4-6</b> Classification Criteria for Persistence and Bioaccumulation	
Property	Classifications
<b>Water Solubility (S)</b>	
Very soluble	$S > 10,000$ ppm
Soluble	$1,000 < S < 10,000$ ppm
Moderately soluble	$100 < S < 1,000$ ppm
Slightly soluble	$0.1 < S < 100$ ppm
Insoluble	$S < 0.1$ ppm
<b>Soil Sorption</b>	
Very strong sorption	$\text{Log } K_{oc} > 4.5$
Strong sorption	$4.5 > \text{Log } K_{oc} > 3.5$
Moderate sorption	$3.5 > \text{Log } K_{oc} > 2.5$
Low sorption	$2.5 > \text{Log } K_{oc} > 1.5$
Negligible sorption	$1.5 > \text{Log } K_{oc}$

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Property	Classifications
<b>Biodegradation</b>	
Rapid	>60% degradation over 1 week
Moderate	>30% degradation over 28 days
Slow	<30% degradation over 28 days
Very slow	<30% degradation over more than 28 days
<b>Bioaccumulation Potential</b>	
High potential	$8.0 > \text{Log } K_{oc} > 4.3$ or $\text{BCF} > 1000$
Moderate potential	$4.3 > \text{Log } K_{ow} > 3.5$ or $1000 > \text{BCF} > 250$
Low potential	$3.5 > \text{Log } K_{oc}$ or $250 > \text{BCF}$

For each of these categories, a score might be given. For example, persistence might be scored 1 through 4 for the four levels of biodegradation listed in Table. Bioaccumulation might be given a score of 1 through 3 based on the three categories of bioconcentration factor. Similar scores could be developed for toxicity. These indices or scores could then be combined, for example, by adding the scores, to arrive at a composite index.

So, there are some then this next 2 slides which just are essentially it may be three or slides what we have a some information available in terms of what is a water solubility how what soil sorption what is the strong sorption what is moderate sorption and all that biodegradation rate bio accumulation potential. So, different numbers are given and based on that we can choose which one kind of does better than the other.

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### Classifying fuel molecules

Compare the soil sorption, water solubility, and biodegradation of three compounds that have been used in gasoline: ethanol, methyl-tert butyl ether (MTBE), and isohexane. Use these data to assess which of the chemicals, if spilled on land, would be more likely to migrate to surface or groundwater. Isohexane is one of the most commonly found molecules in gasoline derived from petroleum. Ethanol is commonly obtained from corn grain, and MTBE was produced in large quantities in the United States from methanol (derived from natural gas) and light petroleum gases (isobutylene).

CCO  
HO-CH<sub>2</sub>-CH<sub>3</sub>

CC(C)(C)OC  
H<sub>3</sub>C-C(CH<sub>3</sub>)<sub>2</sub>-O-CH<sub>3</sub>

CC(C)CCCC  
H<sub>3</sub>C-CH(CH<sub>3</sub>)-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>



And then you can have different types of fuel molecules bigger the molecule bigger the benzene ring very quickly it will degrade very it will be hard to degrade long chain


compounds it does degrade to smaller chain compounds. So, those kind of things are there. So, this is a different types of fuel molecules are present and there is this particular say if you one problem is one kind of sol question has been put forward here that if you compare the soil sorption what is the solubility in bio degradation of three compounds which in gasoline which is ethanol MTBE and isohexane we can assess this chemical espess spilled on land would be more likely to migrate a surface of ground water, depending on solubility and all that is not it.

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*Solution:* Properties for these compounds can be determined through property databases or using methods described in Allen and Shonnard (2001).

Chemical (CAS Registry Number)	Soil Sorption (Log $K_{oc}$ )	Water Solubility (ppm)	Biodegradation (Half-life)
Ethanol (64-17-5)	0.3	Infinite	Days-weeks
MTBE (1634-04-4)	1.3	40,000	Days-weeks
Isohexane (107-83-5)	2.0	14	Days-weeks

The results indicate that petroleum-derived gasoline, if spilled onto ground, is more likely to adsorb to soils than MTBE and ethanol, making it less likely to migrate to water sources and cause water contamination. In contrast, however, MTBE and ethanol have been added to gasoline because of provisions of the Clean Air Act that are designed to reduce emissions of air pollutants. So, while ethanol and MTBE are more likely to find their way into surface and groundwaters than components of traditional gasoline, their use can improve air quality.



So, here are the data which is provided. So, based on this data, since the soil sorption is given to us soil based on soil sorption we will know that higher the soil sorption; that means, more will be the concentration in the soil phase more the water solubility; that means, more has a chances to go into the water phase and in terms of biodegradation if it is quicker; that means, things will degrade faster if it is a longer of life. So, it will take long time to do it.

So, based on that it is if you look at the data the results the petroleum if we have a a spill you most likely that m b that MTBE is a spill of the ground more likely to absorb to soil the petroleum derived gasoline will goes into soil and then MTBE in ethanol again it less slightly because of soil sorption and in contrast how MTBE ethanol is added to the gasoline because of those security using of a machines and all that. So, just to kind of

gives you some idea about based on the soil sorption water solubility you can predict whether things will end up.

So, with that let us kind of wrap this particular module it was and then I hope this kind of gives you a again as I said earlier these we are for many of this topics we have we are able to just do a quick overview of the topic and we will be more than happy to answer any question the discussion forum is already on. So, you can raise questions over there we will be able to answer to your questions and encourage you to look at some of this fate and transport basics. So, there would be other sources of YouTube videos or books and other stuff. So, you; I would strongly encourage you do that because those are very much related to how we do this life cycle in (Refer Time: 32:31) and what does things next to go an inventory.

Thank you and all see you again in the next module.