Environmental Soil Chemistry
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Lecture – 51
Modeling the Fate of Pollutants in the Soil, Risks and Remedies

Welcome friends to this NPTEL online certification course of environmental soil chemistry and today we are going to start our week 11 or module 11 and the topic for this module or this week is modeling the fate of pollutants in the soil, risk and remediations. So basically, we are going to talk about the fate of the pollutants, different pollutants in the soils and what are the risk associated and how to calculate that risk and what are the remedies? So how to cope up with the situation when there is a pollution in the environment?

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So these are the concepts which we are going to cover in this module. First of all, we are going to talk about today the overview of the models. Then we will discuss the classification of the models. Once we complete the classification of the models, then we will be talking about the description of some of the models, some differentiation between different types of models, and then we will be talking about deterministic models.

Once we complete the deterministic model, then we will be talking about transport in heterogeneous media and then we will be talking about sink or source phenomena. Once we complete the sink and source phenomena, then will be discussing the stochastic model and once we cover the stochastic model, then we will discuss what are the problems which are connected with the modeling process of fate of pollutants.

And then we will be talking about model sensitivity, model validation and then we will be talking about the risks and remedial measures. So this is in nutshell the major concepts which we are going to cover. So in the first lecture we will be focusing on the overview of the models and also the classification of the models and if time permits we will also discuss the description of the models.

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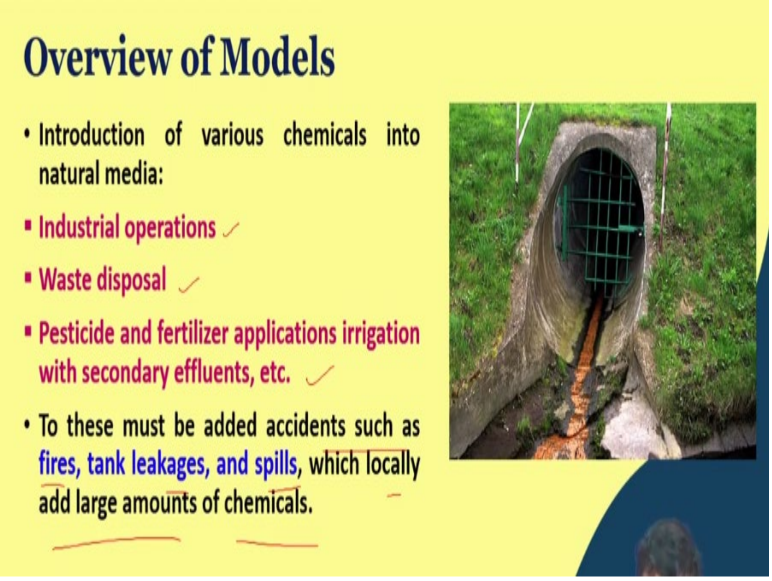

So let us go ahead and discuss you know what is a model and remember whenever we are talking about model especially in this model, this basically modeling the fate of different pollutants in the environment. So if we consider the various chemicals into the natural media, in the natural media you know there are different sources. So, the introduction of various chemicals into the natural media there are different sources, mainly 3 sources.

First of all industrial operations, then waste disposal and then pesticides and fertilizer application and irrigation with secondary effluents, etc. So these are some of the major you know sources of introducing various chemicals into the natural media like soil or water. So, these are the ways through which various chemicals can be added into the soil, however, there is addition of accidents like you know fires, tank leakage and spills.

So when in addition of these different process, there is fires, tank leakage, fires and spills you know which basically locally large amount of chemicals, add different large amount of chemicals into the soil that creates the problem of that excess a bit the existing problem of contamination. So these are different sources and also some additional sources

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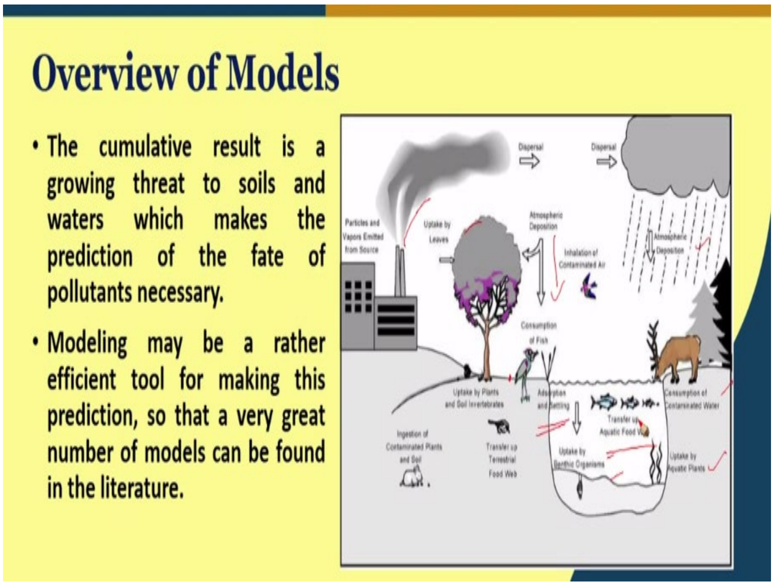

Now, remember the cumulative result coming from all these different sources is a growing threat to soils and waters which makes the prediction of the fate of the pollutant necessary. So once we cover all these different processes and dynamics of pollutants, it is very necessary that we should model the movement and fate of the pollutants in the natural environment. So, modeling may be rather efficient tool for making this prediction.

So that a very great number models can be found in the literature because models are efficient in identifying the fate of the pollutants in the natural media like soil and water. Since you can see these are the movement, this photograph shows movement of different pollutants from within the earth, so basically when there are different types of pollutants they are uptaken by the leaves.

And also the polluted plumes of smokes which are generated by these different industries are showing dispersal and also formation and also different types of atmospheric deposition and when they are deposited they are either consumed by the fish which are present in the water body and there are also adsorption and settling. So up taken by different types of benthic organisms and also transferring of the aquatic food wave.

So, this is how the movement of pollutants may basically occur in the soil and water environment and also you can see there are different types of other transformations also like atmospheric deposition, like consumption of contaminated water by different animals and also from the bottom segments there and up taken by different types of aquatic plants. So, this is how the pollutants move from one place to another place.

And then contaminate the total food chain and also you know move from one place to another place. So, this is why we should focus on the model because model can precisely predict the fate of different pollutants when they move from one place of nature to another place. So this is why we study different types of pollution fate models.

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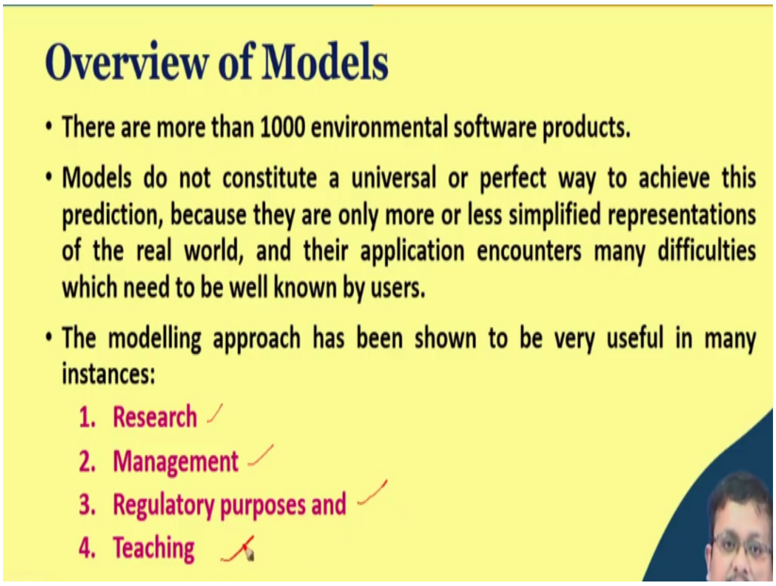

Now, there are more than 1000 environmental software products which are available currently for modeling for modeling the fate of the pollutants and remember that models do not constitute a universal or perfect way to achieve this prediction because they are only more or less simplified representation of the real world and their application encounters many difficulties which need to be well known by the users.

So, we will be discussing these difficulties, what are the drawbacks of the modeling in the later stage of this module when we will be talking about the you know limitations of the modeling. However, the models are the easiest way to represent the real world and the fate of the pollutants. So the modeling approach has been shown to be very useful in many instances.

What are those instances first of all in the form of research, also management and then different types of regulatory purposes and also for teaching purposes. So, we will discuss all these purposes in our coming slides.

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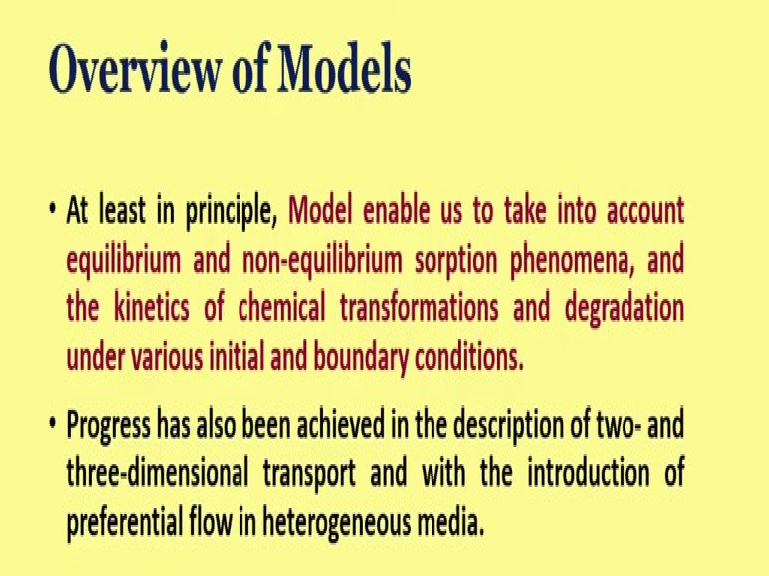

So remember that at least in principle model enable us to take into account the equilibrium and non-equilibrium sorption phenomenon and the kinetics of the chemical transformation and degradation under various initial and boundary conditions. We will discuss that in details in the coming slides.

Now remember that progress has also been achieved in the description of 2 and 3-dimensional transport and with the introduction of preferential flow in heterogeneous media. What is preferential flow, we will discuss in our coming slides.

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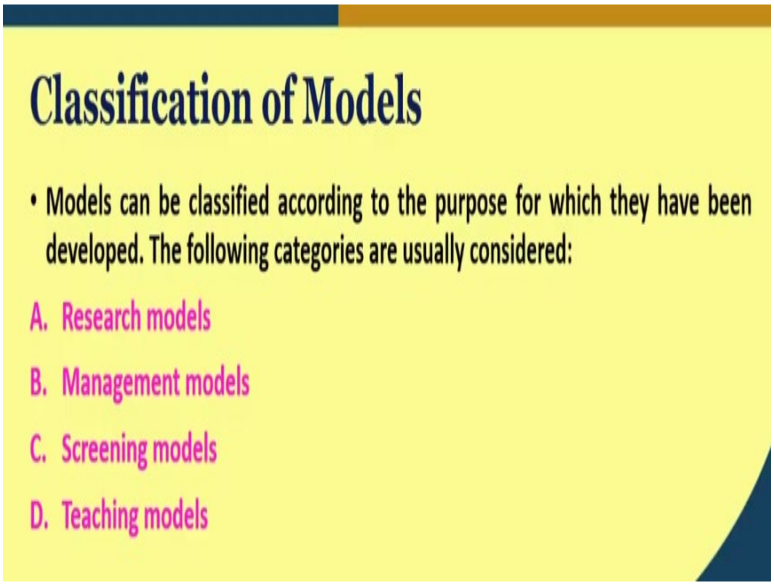

Now let us first see what are the classifications of the models. So while we are considering the classification model, we need to remember that the models can be classified according to the purpose for which they have been developed and the following categories are usually generally considered when you are talking about the purpose of the modeling. So first of all is the research model, then management model.

Then third one is the third category is the screening model and fourth category is the teaching model. So, we will discuss each of them. So, let us first discuss what are the research models.

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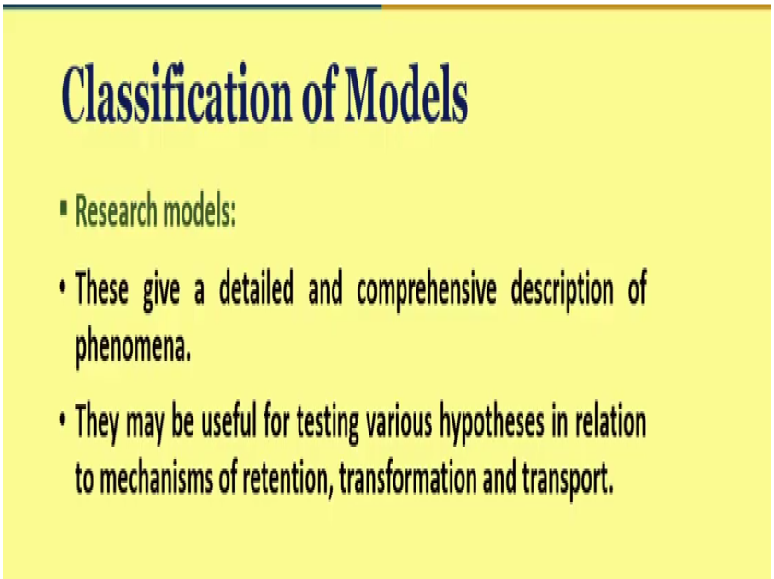

So, research models basically give a detailed and comprehensive description of phenomena. What is phenomena we will also see. Now remember that this is a detailed and comprehensive description of the pollutant fate and they may be useful for testing various hypotheses in relation to mechanism of retention, transformation and transport because this mechanism of retention, transformation and transport play a major role for movement of pollutant from one place to another place.

So to gain a comprehensive knowledge about the full fate of the pollutant you need to have certain hypotheses for testing the mechanism of retention, transformation and transport and these can be done in research models.

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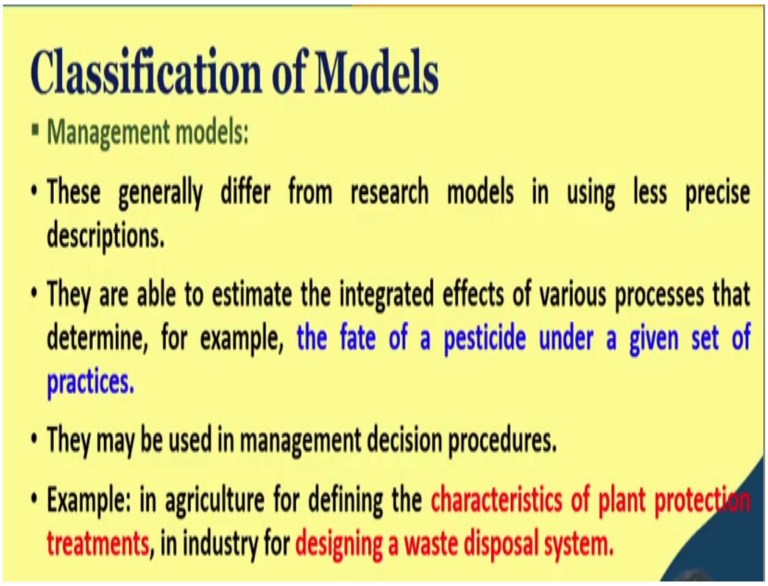

So second category is management models. Now these management models generally differ from research model in using less precise description, research models are more comprehensive and they are relatively more accurate and complex. However, these management models differ from the research models in using less precise description and they are able to estimate the integrated effects of various processes that determine.

For example the fate of the pesticide under a given set of practices. So they may be used in management of decision procedures. So for different types of management, decisions can be taken by using the management models. Remember some of the examples first of all the agriculture for determining the characteristics of the plant protection treatments like what are the different agricultural management which can manage the plant protection chemicals or pesticides in the soil or in the crops.

So also as per as the industrial concern, you know designing a waste disposal system. So, these are all integrated under the management mode. These are all comes under the management models.

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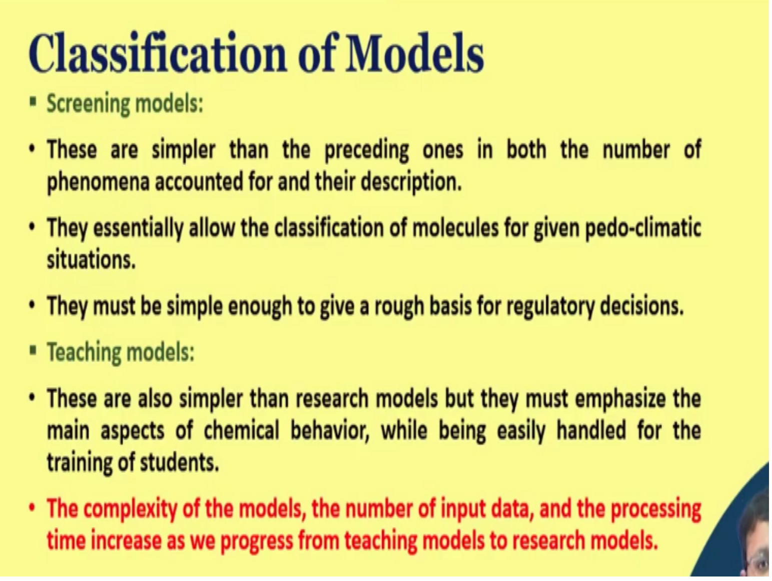

Third one is the screening models. So these are simpler than preceding ones in both the numbers and phenomena accounted for and their description and they essentially allow the classification of molecules for given pedoclimatic situations and they must be simple enough to give a rough basis for regulated decision. So for regulated decision, we generally use the screening models.

The fourth one is the teaching models. So these are also simpler than research model, but they must emphasize the main aspect of chemical behavior while being easily handled for the training of the students. So these teaching models are basically focused on teaching the students and the basically you know emphasize on the chemical behavior. So this is how we differentiate 4 different types of model or classify 4 different types of models.

Now remember that the complexity of the model and the number of input data and the processing time increases as we progress from teaching model to research model. So from teaching model to screening model to management model to research model, the complexity generally increase and also the number of parameters and also the complexity increases.

So as far as the complexity is concerned, research models are more complex than the management models which are more complex than screening models which are further more complex than teaching models. So, we have completed these 4 different types of models or in other words we have completed the classification of the models.

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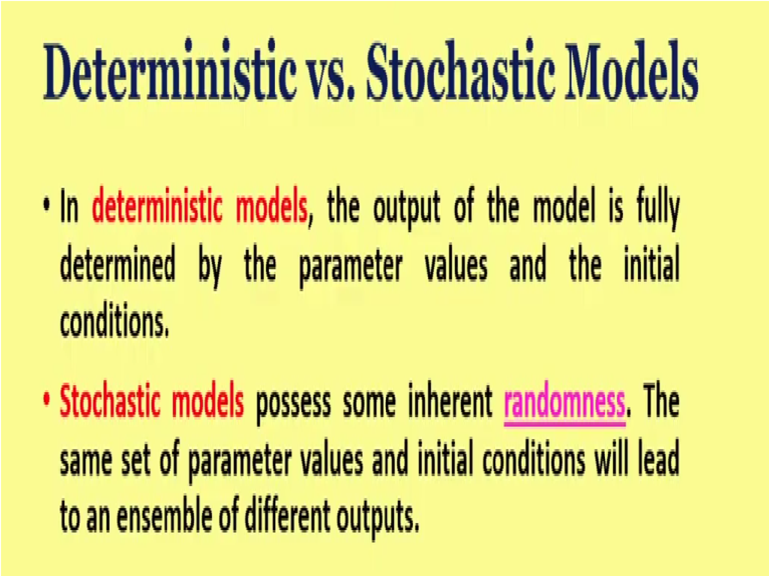

Now, let us see some important model description. Frequently you will come across 2 terms. One is deterministic model, another is stochastic model. We will discuss this both of them in our coming slides in details, but conceptually a deterministic model the output of the model is fully determined by the parameter values and the initial condition and whereas in case of stochastic models, these stochastic models possess some inherent randomness.

So the randomness is the major criteria for stochastic model. Remember that that the same set of parameter values and initial condition will lead to an ensemble of different outputs. So that is why this is the characteristic of stochastic model, it is random. So conceptually this is the difference between a deterministic model and stochastic model.

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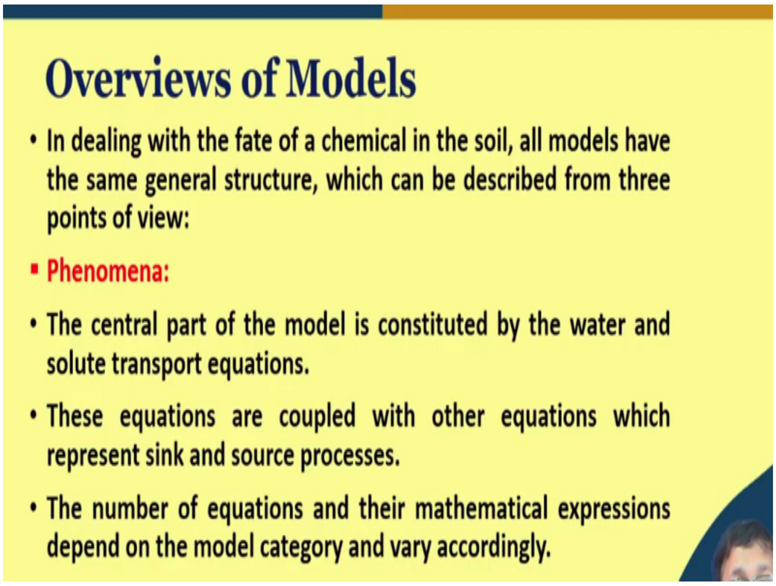

Now if we see the overview of the model, we need to know that in dealing with the fate of the chemical in the soil, all models have the same general structure okay, which can be described from 3 points of view. So if we consider the fate of the chemical pollutant in the soil, there are 3 major structural points. The first point is phenomena. Remember we have talked about the phenomena, now we are going to describe the phenomena.

Now phenomena is basically the central part of the model and is constituted by water and solute transport equations and these equations are coupled with other equations which represent sink and source processes. What are the sink and source process we will also discuss later. So basically, remember that the central part of the model is phenomena which is constituted by water and solute transport equations.

And these equations are coupled with other equation which represent the sinks and source process, sink means from which are originating and source means when they are terminating. Now the number of equation and their mathematical expressions depends on model category and vary accordingly.

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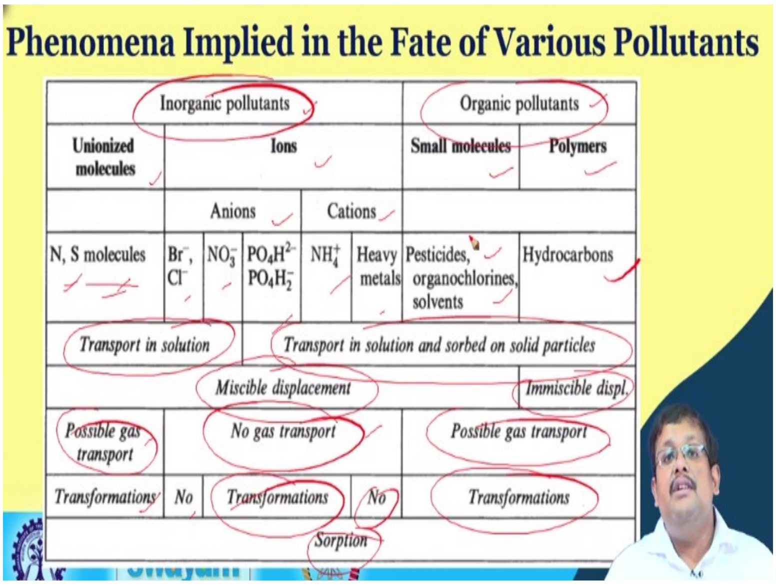

So let us see the phenomena implied in the fate of various pollutants. So this slide shows that there are 2 big categories, one is inorganic pollutant, another is organic pollutants. Now in the inorganic pollutants, there are 2 different categories, one is unionized molecules and another is ions and organic pollutants small molecules and polymers. So among the unionized molecules, you can see nitrogen and sulfur molecules here and among the ions you can see anions and cations.

So among the anions obviously bromide, chloride, nitrate and also different types of primary orthophosphate and secondary orthophosphate ions you can see here and among the cations you can see ammonium and also different types of heavy metals. And in the organic pollutants you can see among the small molecules, pesticides, organochlorines and solvents and in case of polymers hydrocarbons are there.

So, these are some of the classification of the inorganic pollutants and organic pollutants and unionized molecules and ions and small molecules and polymers. Ions can be further subdivided into anions and cations. Now if we see among these different unionized and ions, you know ah these nitrogen and sulfur molecules and bromide and chloride and also nitrate they can easily transport in solution.

However, these cannot be easily transport in the solution like ammonium or phosphates and heavy metals, pesticides, organochlorines, solvents and hydrocarbons. So this is how we can separate them. Now in the furthest stratification, we can see there are miscible displacement and immiscible displacement. So among the miscible displacement, we encompass both nitrogen and sulfur molecules and all these different ions, cations and anions and also pesticides, organochlorines and solvents.

However, hydrocarbons are categorized as immiscible displacement. Now in the next tire we will see what are those which can show possible gas transport and no gas transport and possible gas transport. So you can see here nitrogen and sulfur molecules can show possible gas transport. Similarly, hydrocarbon, pesticides and organochlorine solvents can produce possible gas transport.

However, both anions and cations cannot show any gas transport, be it an anion or cation it cannot show any gas transport. So among this nitrogen in the next tire you can see the nitrogen and sulfur molecules produce different types of transformations, however bromide and chloride they do not show any transformations and nitrate and phosphate show different types of transformations.

Heavy metal does not show any transformation and organic pollutants also produce different types of transformations. However, all of them irrespective of inorganic pollutants and organic pollutants, they are showing the sorption phenomena. So, you can see that this chart gives us a good classification of different phenomena which basically are involved in the fate of various pollutants.

So again, if you start with the inorganic pollutants, they are categorized into unionized molecules as well as ions and organic pollutants are classified into small molecules and polymers and among the unionized molecules basically there are nitrogen and sulfur molecules, anions have bromide, chloride, nitrate and also phosphate and cations have ammonium and heavy metals and small molecules have pesticide, organochlorine solvents.

However, polymers have hydrocarbons. Transport in solution can be shown by these nitrogen and sulfur molecules, bromide, chloride, nitrate, however phosphate, ammonium and heavy metal and also the organic pollutant shows transport in solution and sorbed on solid particles. So, this is how we classify the fate or imply the fate of different pollutants in the natural environment.

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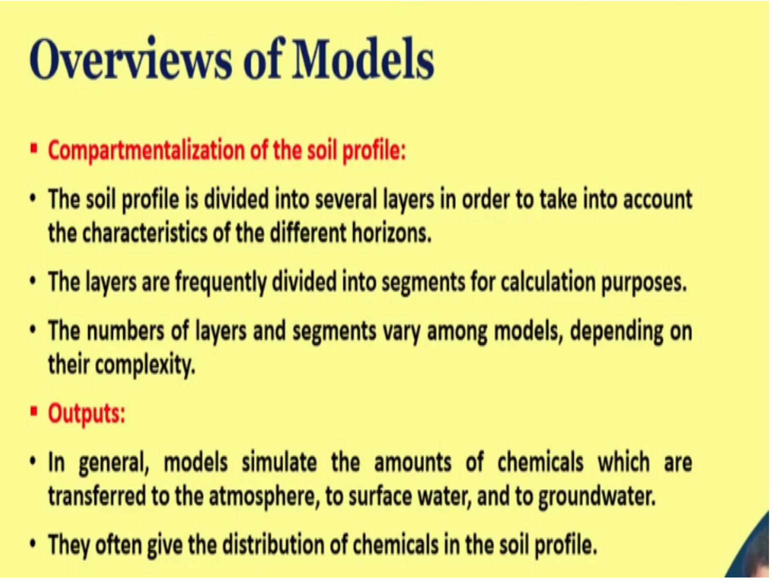

Now we have already completed the phenomena of the model. The next important aspect of a pollutant fate model is compartmentalization of the soil profile. Now remember that the soil profile is divided into several layers in order to take into account the characteristics of the different horizons. You know that soil is differentiated into different horizons. So in this fate transport model the soil profile is divided into several layers in order to take into account the characteristics of the different horizons.

And the layers are frequently divided into segments for calculation purpose, we will see one example and the number of layers and segments vary among the models depending on their complexity and the third important aspect is output. Now remember that in general models simulate the amounts of chemicals which are transferred to the atmosphere, to surface water and to ground water and they often give the distribution of chemicals in the soil profile.

So to understand the distribution of the chemicals in the soil profile, we need to understand the outputs and models simulate the amount of chemicals which are transferred to the atmosphere, to surface water and to ground water.

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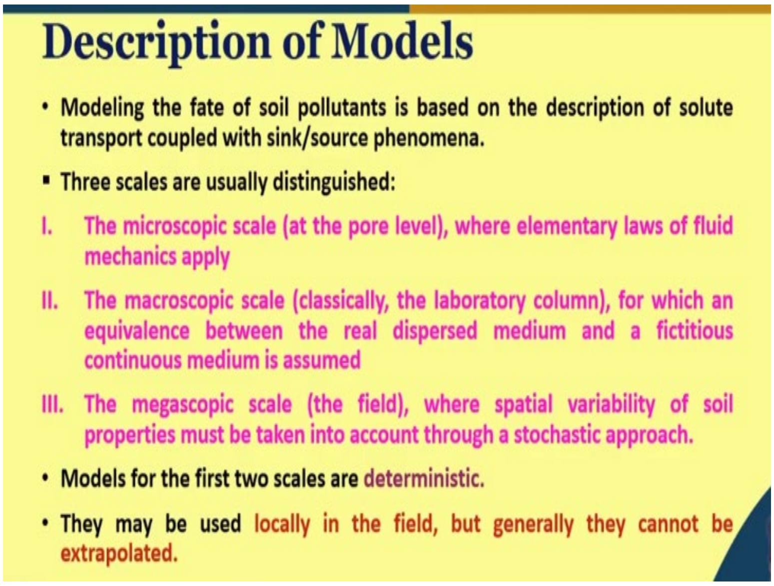

So if you see the description of the model, now modeling the fate of soil pollutants is generally based on the description of solute transport coupled with sink source phenomena. Now the scales are usually distinguished into 3 categories. First of all the microscopic scale of describing a model. So in the microscopic scale, we are basically focusing on at the pore level where elementary laws of fluid mechanisms generally apply.

In the second scale that is called the macroscopic scale classically the laboratory column for which an equivalence between the real dispersed medium and a fictious continuous medium is assumed. So generally, this type of macroscopic scale is performed in the laboratory-based column reaching experiments and the third one is the megascopic scale in the field where special variability of soil properties must be taken into account through a stochastic approach.

So, these are 3 different scales through which we distinguish different types of model. Now remember that models for the first two scales are deterministic in nature, we have already known what is deterministic model. So the first two categories that is microscopic scale and macroscopic scales are deterministic in nature and they may be used locally in the field, but generally they cannot be extrapolated.

Although this first two scales that is microscopic scale and macroscopic scale can be locally applied into the field, however, the model cannot be extrapolated to a new area. So this is the difference between the 3 scales which are used for describing a pollution fate model okay.

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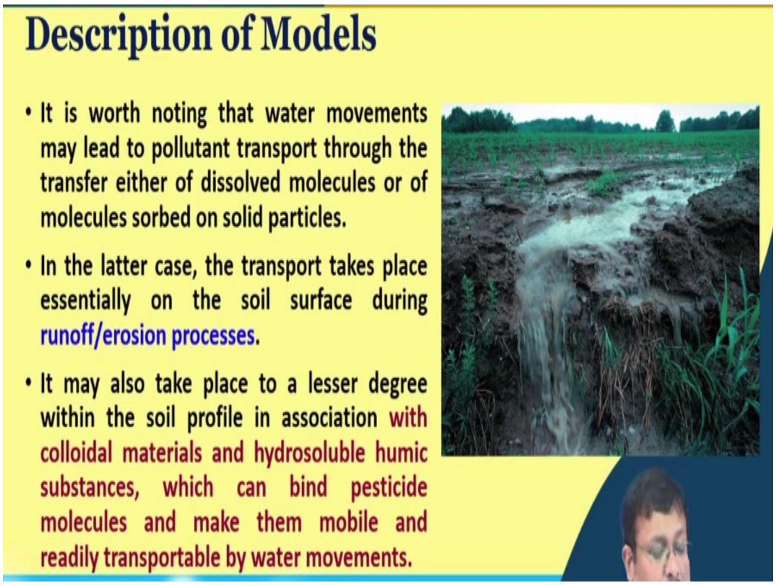

Now remember that it is worth noting that water movements may lead to pollutant transport through the transfer either of dissolved molecules or of molecules sorbed on solid particles. So when there is a transport of water, for example let us take an example of surface runoff. So when there is a surface runoff, the water move and also along with the water the sorbed solved different particles solid particles which are absorbing different types of pesticides or chemicals are also transporting.

So in the latter case, the transport takes place essentially on the soil surface during the runoff erosion process, and third point is it may also take place to a lesser degree within the soil profile in association with colloidal materials and hydrosoluble humic substances. So, the water movement basically when there is a movement of molecules when sorbed onto the solid particles generally happen in case of surface runoff or erosion process.

It may also occur to a lesser degree within the soil profile in association with colloidal materials and hydrosoluble humic substances which can bind pesticide molecules and make them mobile and readily transported by water movement. So in that case also, the chemical move through sorption in the solid particles. You can see one example of surface runoff. I have given this photograph of surface runoff through which the chemicals can move either dissolved in the water or they can be sorbed in the different types of solid particles.

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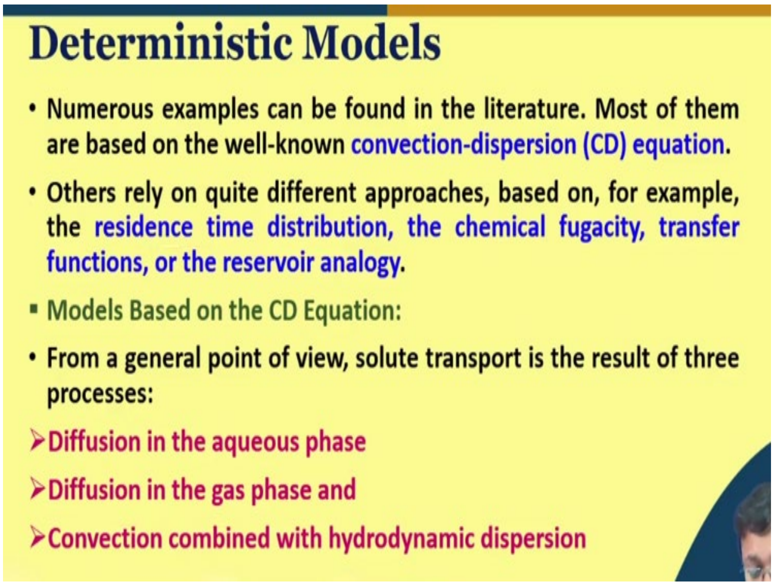

Now numerous examples can be found in the literature among the deterministic models, most of them are based on the well-known convection-dispersion equation. So most of the deterministic model generally rely on this convection-dispersion equation, however others rely on different approaches, for example the residence time distribution, the chemical fugacity, then transfer functions or the reservoir analogy.

So, all the other models are basically you know dependent on these other factors like residence time distribution, then chemical fugacity, then transfer functions or the reservoir analogy. Now remember the model based on the CD equation, from a general point of view, solute transport is the result of, you know in case of model based on CD equation, the solute transport takes a major role and you know solute transport is basically the result of 3 processes.

First of all diffusion in the aqueous phase, diffusion in the gaseous phase and convection combined with hydrodynamic dispersion. So these are the 3 processes through which solute transport occur in the CD model or convection-dispersion models.

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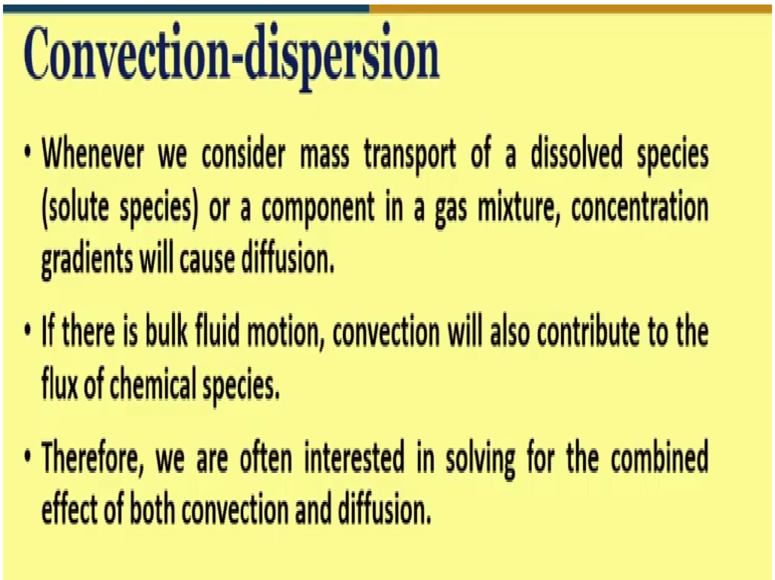

Now what is the convection-dispersion? We need to understand this thing first. What is the coupling of convection-dispersion? Now remember that whenever we consider mass transport of dissolved species which is solid species or a component in a gas mixture, concentration gradients will cause diffusion. Obviously when there is a concentration gradient, there is a diffusion.

Now if there is a bulk fluid motion, convection will also contribute to the flux of chemical species. So when there is a bulk fluid motion, the convection or convective force will also contribute to the flux of chemical species. So therefore, we often integrate this convection and diffusion together to solve different types of basically to solve different types of equation and also for solving the combined effect of both convection and diffusion.

So convection and diffusion are generally combined to describe the solute transfer process in a CD model.

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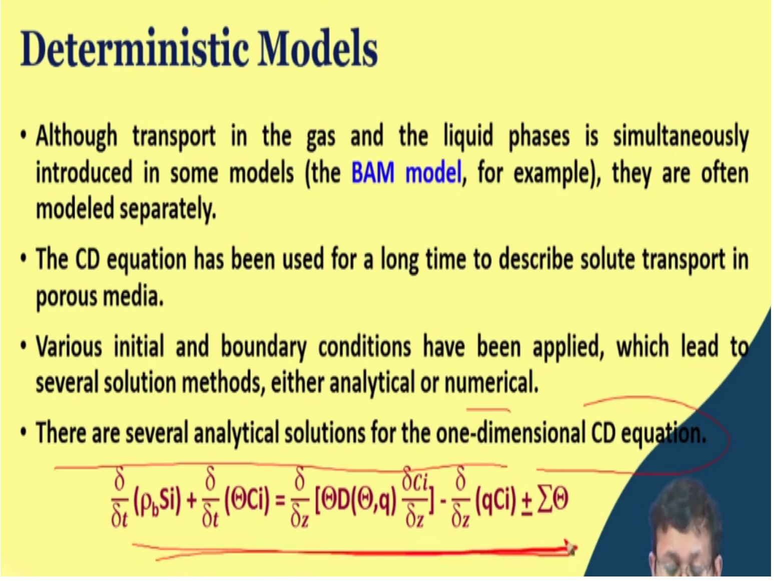

Now in the CD model, although the transport in the gas and the liquid phase is simultaneously introduced in some models like BAM model, they are often modeled separately. Now the convection-dispersion equation has been used for a long time to describe the solute transport in porous media.

Various initial boundary conditions have been applied which lead to several solution methods and either analytical or numerical and this is basically there are several analytical solutions for the one-dimensional CD equation. This is the one-dimensional CD equation. So in this CD equation, let us see what are the individual points.

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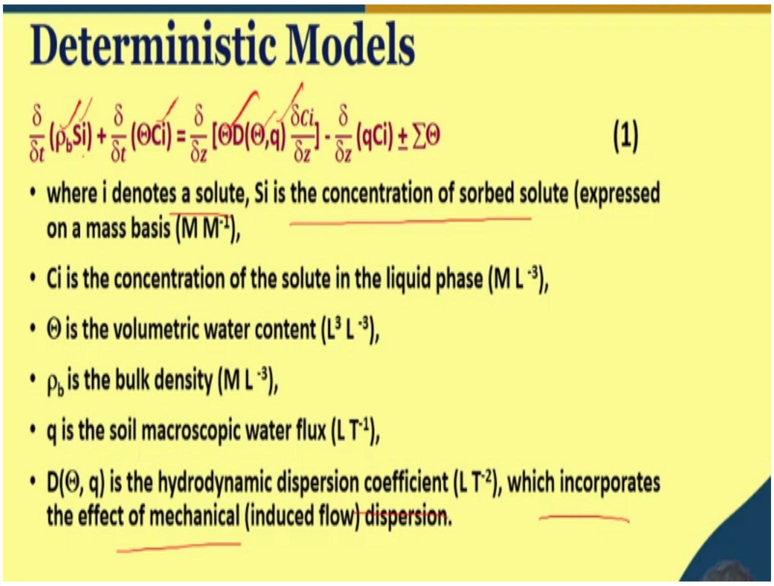

So if you see the equation of the deterministic model in this equation this i stands for a solute. So this subscript i basically stands for a solutes, Si is the concentration of the sorbed solute.

So this Si is the concentration of the sorbed solute, Ci is the concentration of the solute in the liquid phase, theta is the volumetric water content, this rho b is the bulk density and q is the soil macroscopic water flux.

Whereas D theta, q is basically the hydrodynamic dispersion coefficient which incorporates the effect of mechanical or induced flow dispersion. So, this is how we define a CD model equation and let us wrap up this lecture here. In the next lecture, we will see the other types of models and also what are the other different forms of this convection-dispersion models depending on different types of other conditions okay.

So, I hope that you have gathered some knowledge about the pollutant fate models and we will discuss these in details in our next lecture and if you have any question please feel free to email me and I will be more than happy to answer your queries and let us meet in our second lecture of week 11 or module 11. Till then, good bye. Thank you.