ISES Europe Training Series

DoE 3: Exposure Modelling

Module 4: Environmental Exposure Modelling

Hello everybody, this is Natalie von Goetz and I will present to you the module 4 of the domain of expertise 3 exposure modelling and this is part of the ISES Europe training series.

First of all, some disclaimers and the overview of all training videos. And now, where are we? You have probably already heard the modules 1 to 3, and now we will talk in module 4 about environmental exposure modelling. My name is Natalie von Goetz. I am working as a project leader at the Swiss Federal Office of Public Health and also as a lecturer for the Federal Institute of Technology, ETH Zurich, where I have formerly also been a group leader for human exposure modelling, and even before I was a laboratory manager for BASF. My education is in chemistry. I did a PhD in natural sciences where I already did some exposure modelling.

Now again, a disclaimer, and here are your learning objectives: By hearing this module, we want you to understand the principle of environmental exposure modelling and the concept of compartment models and their use. We want you to be able to describe tiered approaches in environmental exposure modelling and to explain environmental exposure modelling for pesticides.

The content of today is general principles, then I will describe the environmental processes and how they are described by mathematical formulas. And then I will give you two different examples for exposure modelling under different legislations. These are legislations that differ in the availability of data. REACH is a legislation where there is not so much data available. And for pesticides, there is a lot of data available. Then I will give you a summary.

First of all, the general principles: Exposure modelling for environmental risk assessment focuses on environmental compartments and representative organisms. So what are environmental compartments? They are the different environmental media that we have. And for these environmental media and the organisms that live in the respective environmental media, a risk is assessed by, again, combining exposure and effect by comparing these two. The effect you have already heard about in the domain of expertise two, and since this is a lecture series on exposure assessment, I will not further go into the details here. Instead, we will look into more detail into the different processes that govern the exposure of substances in the environment.

Now, we have the degradation and metabolization, which reduces the concentration of the substance overall. Then we have partitioning, which means the transfer between different environmental media, like, for example, between water and soil, which also serves to reduce the concentration in one medium, but it increases the concentration in another medium. And then we have transport, which means that a substance is transported into different areas, which also reduces the concentration at a specific locality, but then results in concentrations in other places of the world.

So which environmental media are we looking at? We have, obviously, the soil, then we have water, and this is subdivided into surface water and groundwater because of the different processes that lead to the concentrations in the groundwater and the surface water. Then we have the sediment and also the air. PEC means predicted environmental concentration, so concentration that is calculated and not measured.

Coming to the environmental processes, I would like to start with the compartment models for degradation and metabolism. Compartment models or box models are very convenient to describe different processes in the environment. We are thinking of a compartment as one entity with a defined concentration of a defined substance in a specific medium. For degradation, we assume that there is a box or compartment with only the parent substance, which is the substance that we first wanted to look at. And then we have a degradation into metabolite one and metabolite two with the degradation rates k1 and k2. And here we assume for simplification that the degradation follows first order rate law. If we assume this, we can easily establish differential equations that help us calculate the concentration in each of the different compartments after a certain time for each time point.

The graphical representation can look like this. You can check compartment one which is the parent, you see we start at 100% and this goes down in time. And for the first metabolite here, which is the blue line, we have a steep increase and then also a decrease when it further degrades to metabolite two, which then builds up. This is the green line. And then in the end, we have the CO2, carbon dioxide, which is the end product of most substances that we know.

These compartment models can also be used to model the process of partitioning. We can assume that a substance is only in water and this compartment here is the substance in water. And the other compartment to the right is the substance in soil. And we have then the process of adsorption and the process of desorption with specific adsorption and desorption constants. Also here, we assume linear adsorption so that we can establish this rate law. And in equilibrium, where we don't have any change of concentration in the compartments, we can then further derive the equation to the right and define a constant Kd that describes the behaviour of the substance when it comes into a system of water and soil. And this is very helpful in the description of the behaviour of substances in soils. Also, since one knows that the organic carbon content plays a major role in the adsorption of substances, because they mainly adsorb to the organic carbon, this Kd value is normalized by the content in organic C of the soil. And the resulting KOC, the distribution coefficient or absorption coefficient, is then used in models to describe the partitioning between water and soil of a substance. There are further sorption models, but since this is an introduction, I only want to mention them here without giving further details. But the principles are mainly the same.

We can also move this further. We have different other compartments. We have air, we have also a possible source, Q, and we have biological tissue. And by help of these different compartments, we can then make a model for the whole reality. And we can also derive then constants that describe the partitioning between all the different compartments. One of the constants and one of the laws has a specific name, which is Henry's law that describes the partitioning between air and water. The others have no names, but it is the same principle. And based on these ideas, you can construct multimedia models like the one to the right that is depicted here and also contains a compartment for oceanic surface water. These multimedia models have a broad applicability in environmental fate modelling. They can also be used to describe transport via air. If you are considering this unit that I just showed you multiplied into many additional units and put one after the other, then you can also describe with these units the transport via air. Some examples of these models include the model SimpleBox, which is often used in the EU. RADAR, BETR Global, ClimoChem are other multimedia models that use slightly different assumptions, but essentially work by the same principle.

After these preliminary introductions about the concepts that are being used in environmental exposure modelling, I would like to give you two examples, one example being the REACH legislation and one example the pesticide regulation.

Coming to the REACH legislation, this is a comparatively new legislation. It has entered into force 2007 and is applicable to industrial substances, but also to substances for end users. It is mainly applied when no other specific legislation applies, like for food, for cosmetics, food contact materials, where there are specific legislation, REACH is not applied. The responsible agency is the European Chemicals Agency. And if you are interested further, you can have a look at their website, they have many materials there. I will not go into the details because there is a complete domain of expertise and legislation. But I thought it is necessary to have this in mind when I talk about the environmental fate modelling that is required under the different legislations. Under REACH, a primary focus is on surface water, and there are several requests for environmental modelling. I will only quickly explain one of them, which is the request that for every industrial site, a predicted environmental concentration has to be calculated.

And this is then done by considering not only the concentration that is resulting from the emissions of the respective site, but also taking into account the background concentrations. And these background concentrations are calculated with multimedia models, where one continent concentration is used as input to the multimedia model, and then the PEC resulting from the multimedia model is used to calculate the overall local concentration. There are many simplifying assumptions. For example, immediate and complete mixing is assumed and evaporation, degradation and sedimentation is not considered. The complete mixing makes it a little bit less conservative, but on the other hand, degradation is disregarded. So overall, one has the feeling that they deliver a reasonable estimate for the concentration.

The model equations that are being used then for the PEC local water, which has to be calculated by legislation, is that you can use the PEC regional from the multimedia model and add it up to the C local water that each industry site has to calculate for themselves from the C local effluent, which means the emission into the surface water. And then there are some correction factors applied.

I am coming now to the environmental exposure modeling for pesticides. Pesticides legislation has a long history, dates back to the 1970s. Currently, it is based on the regulation 1107 2009. It is applicable only to pesticides and the responsibility lies with DG Sante and the European Food Safety Agency.

And for pesticides legislation, for each pesticide, a whole dossier, which is very comprehensive, has to be submitted. That includes, for example, environmental fate, laboratory experiments and field experiments for the pesticides and also extended human toxicity experiments and environmental toxicity experiments and also analytical methods. The data requirements are much, much more extensive than for the REACH legislation, where the requirements depend on the tonnage that is sold in Europe. But for pesticides, for each pesticide, the same dossier is requested regardless of the tonnage, and this is quite extensive. So for pesticide exposure assessment, there are a lot of data available and these exposure assessments also have to be done by the industry submitting the Dossier. Here, all environmental compartments are assessed, unlike in the REACH legislation where mainly surface water is assessed.

This equation here for the initial PEC includes the application amount A, and then there is some correction factor for interception by crops. Further, there is a factor that takes into account that the substance enters only a certain depth of the medium and then also a correction with the density. So in the end, the PEC-ini describes the concentration of substance in the volume that is assumed as a distribution volume for the substance. Starting from this initial PEC, there can be a degradation. This is why there is a time-weighted average predicted concentration, which is used as a higher tier approach. This time-weighted average PEC is just the area under curve divided then by the number of time steps considered, so it's just a mean value for a predicted concentration over a certain time.

And here's something about the wording that is used in pesticides legislation. So the risk index that is used in pesticides legislation is the toxicity exposure ratio, the TER. And the toxicity values that are being used are LC50, the lethal concentration, where 50% of the organisms die and the no effect concentration NOEC. These are compared then either to the initial PEC or the time-weighted average PEC. Also here a tiered approach is being followed because as a tier one only the PEC initial is compared to the LC50, but with a safety factor of 1000. So if this toxicity exposure ratio is lower than 1,000, this means that there might be a risk. And as a second tier, the calculation with the NOEC and the PEC-twa can be done. And this calculation that I showed with the application amount, this can be used either for soil or also for the surface water.

Only that for surface water, we have to consider that there are different entry paths into the surface water. There is drift, which means that the mist from the application can be transported via the air into the surface water. Then there can be runoff, which means that the substance is adsorbed onto soil in an applied area, and then the soil is transported by heavy rainfall into the surface water. And then there can be drainage, which means that there are drainage pipes in very wet soils where the water of the rain is accumulated in these pipes, and they directly lead the substance then into the surface water. After considering all these pathways, the calculation is done in the same way as described up here, only that you assume a different density and a different application rate, obviously, and also a different depth of entry.

There are several models that can be used for surface water modeling, but
since this is an introductory course, I will not go into the details. If you are interested in reading further, you can visit the website of the FOCUS DG Sante group.

Coming to groundwater modeling, here also dedicated models are available because it is quite complex what happens to a substance when it enters the soil and leaches into the groundwater. The most important parameters from the substance are the KOC values, so the partitioning between water and soil, and the DT50 value, so the degradation of the substance. On the other hand, what is very important is the scenario data, and here the weather, the rain and temperature, and also the soil, the soil profile and the soil properties. The models that are being used are based on differential equations for the water and heat flux in the soil, for example, the Richards equation. And what is then done by the models, they are calculating the mean concentration in one meter depth below the surface of the soil. This is a convention that is being used because mostly the groundwater level is deeper than one meter depth.

Regarding the exposure scenarios for pesticides, you can imagine that in Europe we have quite different soil types and we also have very different weather conditions. What has been done also by the focus group, which is a group from academics, industry and administration who came together and agreed on reasonable scenarios. They have defined these nine scenarios over the whole of Europe with different combinations of rainfall, temperature and soil type. And apparently these scenarios match the European conditions quite well: The green dots that you see is show that these are covered by the focus scenarios. The red ones are scenarios that are not covered. So here the respective national agencies have to check whether the assessments are conservative enough or not.

Also for groundwater, a tiered approach is being followed. So as a first tier, you have these scenarios that I just explained. Initially, you are only doing the groundwater assessment by means of modelling. You are not using any tests in the field. And if you see that there are problems with the assessment, you can do a modelling with refined parameters or refined scenarios, so very specific to the crop that you want to use the pesticide in. And then there are different other possibilities for a tier three. For example, you can then also do some experiments to check whether the model is right.

Coming to the summary of this module, I hope that I was able to convey that models for environmental exposure are based on general principles. They often assume steady state for simplification, but they have also been shown that they work. This helps to give a first impression so that not so much so resources are spent and still that the complexity of the environment is being assessed. Then, depending on the legislation, for example, I gave you an idea about what is done for pesticides and which different data sets are available for modelling, and that the models have different levels of detail. Also, different legislations may focus on different environmental compartments depending on the emission scenario.

With this, I want to close and wish you well and hope that you are following up with the module five so that you have then heard the whole domain of expertise. Thank you for your participation and attention.

