APPLIED ENVIRONMENTAL MODELING EXAMPLE

Environmental modeling is often used to illustrate and predict exposure concentrations, identify major transport mechanisms, and estimate chemical persistence. If necessary, we might consider using environmental fate modeling to examine the pathways of dioxins through the aquatic environment of the Mekong River in the vicinity of our hypothetical KL pulp and paper mill. Modelling outputs will supplement the results of the ecological risk assessment (ERA) and environmental impact assessment (EIA) completed for the project and collaborate the results of environmental effects monitoring (EEM) monitoring undertaken in the vicinity of the mill.

The following brief example of environmental modeling is intended to provide some background on the components and steps involved in modeling a system of interest.

An environmental fate model requires two sets of data:

1. A description of the evaluative environment i.e., how much water? how much air?
2. Information about the properties of the contaminant being modeled.

THE EVALUATIVE ENVIRONMENT

The environment can be described as a number of compartments, all interacting with one another, depending on their location and properties. For example, continuous compartments are always in contact with one another (i.e., air and soil, water and sediment). There are also non-continuous compartments, which consists of many particles that may not always be in contact. Examples of non-continuous compartments include fish swimming in water, suspended particles in water, and the aerosol component of air. Figure 1 shows typical four- and eight-compartment evaluative environments.

Air

The lowest layer of the atmosphere is the troposphere, which extends from the surface of the earth to approximately 10 km. In most large-scale models, the troposphere is assumed to have a depth of 6 km. A model concerned with local effects (i.e., air quality above a city) might select an arbitrary air depth of 1,000 metres. Site-specific meteorological information might refine that value further.

Aerosols

The atmosphere contains many particles, including water, soot, dust and smoke, which play an enormous role in environmental fate modeling, since many chemicals can bind to atmospheric particles. Typically, a rural area would have an aerosol concentration of 5 μg/m^3, while a polluted urban area would have a concentration of 100 μg/m^3. The

Figure 1 Evaluative environments

amount of aerosols per cubic meter of air is often expressed as a volume fraction to reduce the amount of mathematics; a typical volume fraction is 2×10^{-11}. As a result, an air volume of 6×10^{9} m^3 is assumed to have 0.12 m^3 of aerosols. This number can be refined with site-specific information (i.e., smog readings from a local air quality monitoring station).

Water

Although 70% of the earth's surface is covered by water, most models only consider water close to shore and within 100 m of the surface. For the purpose of the model, the water is assumed to be pure (i.e., not salt water, brackish or containing electrolytes), although suspended particles (i.e., very small pieces of organic or mineral material) are considered. The volume of water should be reflective of site-specific conditions (i.e., a model considering a mountainside would obviously contain less water than a lake model).

Suspended Particles

Particles in a water column play a key role in the fate and behaviour of contaminants. Very clear water might have a suspended particulate concentration of 1 g/m^3, while muddy water may contain over 100 g/m^3. As with aerosols, the amount of suspended particulates in water is usually expressed as a volume fraction (e.g., a typical volume fraction is 5×10^{-6}).

Fish and Aquatic Biota

Fish are valuable for commercial fishing, as well as for local sustenance. Fish also tend to bioconcentrate or bioaccumulate contaminants, and are therefore useful indicators of water quality. A typical volume fraction of fish in a water body is 10^{-8} – we ignore other biota in the waterbody (i.e., benthic invertebrates, algae) to focus on the fish.

Sediments

Sediment on the bottom of a lake, river or ocean is a complex mixture of organic and mineral material that is constantly changing through resuspension and deposition. In general, we are most concerned about the active layer at the water/sediment interface, which is generally well-oxygenated, contains high amounts of organic material, and is home to diverse communities of benthic organisms. The typical composition of the active layer is 5% particles and 95% water. Sediments often act as a sink for contaminants, as they bind to sediment particles and are buried by layers of deposited material.

Soil

Terrestrial soils are also a mixture of organic and mineral materials, along with pockets of air and water. A typical soil may consist of 50% solids, 20% air and 30% water.

A summary of typical volumes, densities and compositions for each of the eight compartments is provided as Table 1.

CHEMICAL PROPERTIES

The physical properties of a contaminant govern its behaviour and fate in the environment. Many chemical properties measure the ability of a chemical to transfer from one compartment to another, and are referred to as partition coefficients. Although a detailed examination of all properties is beyond the scope of this

Table 1 Default compartment properties values in a typical evaluative environment

COMPARTMENT	VOLUME (m^3)	DENSITY (kg/m^3)	ORGANIC CARBON OR LIPID CONTENT (%)
Air	1×10^{14}	1.185	-
Water	2×10^{11}	1000	-
Soil	9×10^{9}	2400	2
Sediment	1×10^{8}	2400	4
Suspended particles	1×10^{6}	1500	2
Fish	2×10^{5}	1000	5
Aerosol	2000	2000	-

lesson, several key physical properties should be considered:

- Vapour pressure – the tendency of a chemical to partition into the atmosphere from a liquid form (i.e., a beaker of gasoline will 'evaporate' into the air).Water solubility – the tendency of a chemical to partition into water from a solid form (i.e., a sugar cube will dissolve when placed in water).
- Henry's Law constant – the tendency for a chemical that is dissolved in water to transfer into the air (i.e., essentially, a combination of vapour pressure and water solubility). A chemical with a high Henry's Law constant will tend to move from water to the air, a chemical with a low Henry's Law constant will tend to remain in aqueous media.
- Water-octanol partition coefficient (K_{ow}) – the tendency for a chemical to partition into lipids (i.e., fat). A chemical with a high K_{ow} is more likely to accumulate in fish than a chemical with a low K_{ow}.

Other chemical properties, such as boiling point, melting point, and density may also be important.

The K_{ow} is the most important property for describing the fate and movement of a contaminant in the environment. It is a measure of hydrophobicity, or the tendency of a chemical to 'hate' water. A chemical with a high K_{ow} is referred to as 'hydrophobic' (i.e., the chemical is more likely to partition into an organism), while a chemical with a low K_{ow} is referred to as 'hydrophilic' (i.e., water-loving; the chemical is more likely to remain in the water). If a dissolved chemical is hydrophobic, it will tend to bind to the organic carbon portion of sediments (i.e., either bottom sediment or suspended particles), or will tend to partition into the tissue of fish and other aquatic biota. A good example of a hydrophobic compound is mixing oil and vinegar – the oil 'hates' the water in the vinegar and therefore forms globules of oil instead of dissolving evenly.

A typical organism (e.g., a fish) consists of many different tissues, including muscle, liver, gills, etc. For the purpose of modelling, we can simplify the fish and assume that it is simply a box, containing mostly water and a little bit of fat. A typical fish usually contains about 5% lipids. The K_{ow} describes the movement of a chemical between the surrounding water and the 5% lipid part of fish tissues.

THE MODELS

Models take many different shapes and sizes, with varying degrees of complexity and geographic coverage. One common type of model uses the principle of mass-balance as a basis to predict the fate and behaviour of contaminants. Mass-balance is based on the idea that the entire mass of contaminant must be accounted for in the model – the amount of contaminant released in effluent or spill must equal the amount of contaminant that eventually ends up in different parts of the environment. The challenge of the mass-balance approach is deciding how to subdivide the environment in many different compartments, and then describe a mathematical relationship that explains how contaminants move from one compartment to another.

A basic approach to modeling follows the principle that the best method is often the most simple. In many cases, increasing the complexity of the model does not result in an increased certainty about what the model is telling you. Three different versions of a mass-balance model are presented below.

Level I

The Level I model (Figure 2) simulates the release of a fixed quantity of a substance and makes many assumptions to simplify the mathematics, including:

- Chemicals do not react or degrade over time
- No transport occurs between different compartments, except what would be expected according to the chemical's properties
- No input or output of the chemical occurs except for the initial amount.

The model also assumes that the distribution of the chemical is in equilibrium (i.e., a great deal of time has passed to allow the chemical to fully partition into the various compartments). These assumptions make the Level I model impractical for modeling an actual project site, but do allow scientists to explore the environmental fate of a new chemical prior to its release.

Level II

The Level II model is more complex than the Level I, as it assumes that a chemical is input at a constant rate over time (Figure 3). The Level I model assumed that the contaminant release was a one-time only event.

The Level II model also allows for a chemical to leave (i.e., output) from the evaluative environment through advective transport (e.g., large-scale transport of the chemical in a river). The model assumes that input and output rates are equal (i.e., the model is at steady-state conditions). As with the Level I model, the Level II assumes that enough time has passed to allow the chemical to fully partition in the different compartments (i.e., the model is at equilibrium)

The Level II model is more realistic, and its parameters can be modified to reflect site-specific conditions.

Figure 2 Level I model

Figure 3 Level II model

Level III

A Level III simulation is more complex and realistic than the Level II model. The Level III model assumes that a chemical is being added and lost at the same rate (i.e., the input and output are equal; the model is at steady-state conditions). However, the Level III model does not assume equilibrium conditions, and is therefore more reflective of real-life conditions. This means that the user can specify which compartment is getting the input of chemical (i.e., 100 kg/hour to the air, and 900 kg/hr to the water, as shown in Figure 4). The transport rates between compartments are also included, such as sedimentation, water flow, air-borne deposition and soil run-off. Reaction and degradation rates are also included. The model also calculates a chemical's persistance and residence time.

The Level III model provides a realistic description of environmental fate, including the important degradation and advection transport losses and between-compartment transport processes. The distribution of the chemical between compartments depends on how the chemical enters the system.

ADVANTAGES AND LIMITATIONS OF ENVIRONMENTAL MODELING

It would be wrong to assume that a model, no matter how complex, can completely describe the fate and behaviour of a chemical such as dioxin in the real world. A model is not a substitute for actual measurements of chemical concentration. However, a good model may reveal more about a particular chemical's behaviour than we might otherwise learn through conventional (i.e., limited number) sampling techniques.

The model is only as good as the information it contains. For example, many of the model calculations rely on the chemical's properties, such as vapour pressure and water solubility. These properties are usually measured at 25ºC; but the real world has varying temperatures. The selection of compartment volumes also plays a huge role in how the model works; can a static value for the volume of fish in a river really represent changes due to annual migration?

The models presented in this lesson make several major assumptions. For example, the Level I and II models assume equilibrium conditions, where the chemical is fully partitioned into all compartments. All the models assume steady-state conditions, where the inputs equal the outputs. In real-life, these conditions almost never occur. For example, the flow rate of a river changes seasonally, changing the concentration of contaminants in the water. The amount of effluent from a pulp and paper mill might change depending on how much paper is being produced. Contaminants might come from multiple sources, instead of from only the source being modeled.

Finally, an eight-compartment model cannot completely describe the complexity of the real world. There are food-chain dynamics that are ignored by assuming the biota compartment only contains fish; terrestrial organisms and plants were completely ignored.

So why use a model at all? The model provides many advantages, but the best reason to use a model is that you can predict how a chemical might behave before any pollution occurs. For example, for the KL pulp and paper mill example, you might predict (using the

Figure 4 Level III model

Level III model) that 96% of the 2,3,7,8-TCDD will end up in the river sediments, and not in the water. This would provide valuable information for designing a monitoring program. Additionally, you could run the model many times, each with a different amount of 2,3,7,8-TCDD (i.e., representing different effluent concentrations) until you found one that kept the final concentration in the water below a safe concentration. Modeling can be used to simulate different effluent treatment technologies, or help decide what conditions to place upon project approval.

Many models have been developed, from the equilibrium partitioning models discussed in this lesson, to groundwater flow models, to food chain models. Models can be as complex or as simple, and as site-specific or generic as needed. Overall, modeling is simply another tool for environmental managers and decision makers to use in monitoring and assessing proposed projects.