EPA
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Exposure Assessment (EXA)
Course Series

Monitoring and Modeling Strategies

Reading Packet

EXA 405



EPA's Risk Assessment Training and Experience (RATE) Program

EXA 405: Monitoring and Modeling Strategies

READING PACKET

Exposure Assessment (EXA)
Course Series

EPA's Risk Assessment Training and Experience Program

EXA 405: Monitoring and Modeling Strategies

The objective of this module is to provide an overview of means to assess sources and exposure media through the use of monitoring and modeling. This module will build on the earlier modules on exposure scenarios (EXA 403) and fate and transport (EXA 404) by introducing the participants to concepts of monitoring and modeling. In the first half of this course, monitoring study design will be described. The course will cover concepts of laboratory quality, including the important concept of the detection limit and how to handle "censored" data. In the second half, students will learn about environmental modeling, with discussion covering development and implementation of a modeling strategy, model types and limitations, and model evaluation. Several environmental models will be presented as examples.

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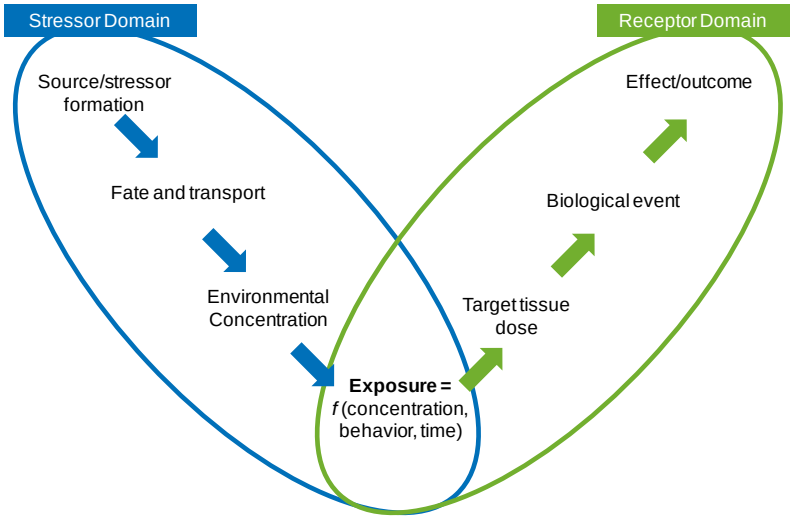
1. INTRODUCTION TO MODELING AND MONITORING STRATEGIES

The combined use of monitoring data and modeled results is a valuable approach for quantifying exposure for human health risk assessment. This course focuses on the basics of **monitoring**, including designing a monitoring study, collecting and evaluating data, and using these data in exposure assessments. In addition, the course covers metrics used in interpreting monitoring data and data quality. This course also explores **modeling** environmental concentrations, including selecting an appropriate model, applying and using the model as part of our exposure assessment, and evaluating the model. The types of environmental concentration models frequently used by EPA in risk assessment are also discussed.

To understand where monitoring and modeling fit into exposure assessment, it is useful to refer again to the source-to-effect continuum shown in Figure 1. Environmental monitoring can provide information on environmental concentrations of a stressor, and it can also assist in evaluating source/stressor formation and fate and transport. These activities can feed into any of the four steps on the left side of Figure 1, including estimating the environmental concentrations to which people are exposed. Environmental models can help to inform the fate and transport and the environmental concentration components of the left side of the source-to-effect continuum (Williams et al., 2010).

Figure 1. Source-to-Effect Continuum



Other models will be discussed that can be used to model exposures at the nexus of the two halves of the continuum (taking into account human behavior and time); some of these models were introduced in EXA 402. A third category includes models that estimate dose. These models will not be covered in this course.

2. MONITORING STUDY DESIGN AND DATA GATHERING APPROACHES

There are many reasons for environmental monitoring of pollutants. This course focuses on monitoring conducted to better understand human exposure, and specifically on monitoring of concentrations of chemicals in environmental media.

Environmental monitoring provides the concentration terms in relevant media for calculating exposure and dose at a specific location and for a given time period. These data can be especially useful when conducting a site-specific risk assessment. Monitoring also allows us to identify and fill data gaps. In other words, by monitoring pollutants in environmental media, we are better able to know what is in the environment and where people might be potentially exposed (U.S. EPA, 1989).

2.1 Study Design

We begin monitoring by designing a study or sampling plan or, if we are using data collected previously, we begin by reviewing and evaluating the study design.

Design Considerations

There are some important considerations when designing or evaluating a study that involves monitoring data.

- Why is or was the study conducted? What question(s) is or was the study looking to answer?
- What is the scope of the study?
    - We define the scope in terms of what will be monitored, where it will be monitored, and when it will be monitored. The answers to these questions help us identify the media of concern; the relevant geographic scale and the extent of contamination; and the timescale (for example, whether exposure is likely to be acute or chronic).
- How accurate must the measurements be to meet the intended uses? How is the monitoring program limited by resources, and what is the most effective use of those resources to fulfill our goals? In other words, what is the appropriate level of detail?

Once the purpose, scope, and level of detail have been defined, we can determine our specific approach to measurement (U.S. EPA, 1992).

Components of a Monitoring Plan

In designing or reviewing a monitoring plan to support an exposure assessment, we need to consider site history, site location, and potential exposure scenarios that might direct our data collection. Based on this information, we can develop a conceptual model of exposure, identify data quality objectives, define our sampling rationale, and choose our data evaluation methods.

Typically, the geographic domain is important to our monitoring plan because it helps us to identify the contaminated media, the potential fate and transport between media, and possible exposure pathways/routes. The site history might offer additional information that is important to our exposure assessment. If previous assessments have been conducted at a site or for similar exposure scenarios, these could offer insight into the current assessment and also provide metrics for comparison. We also need to consider the operational history

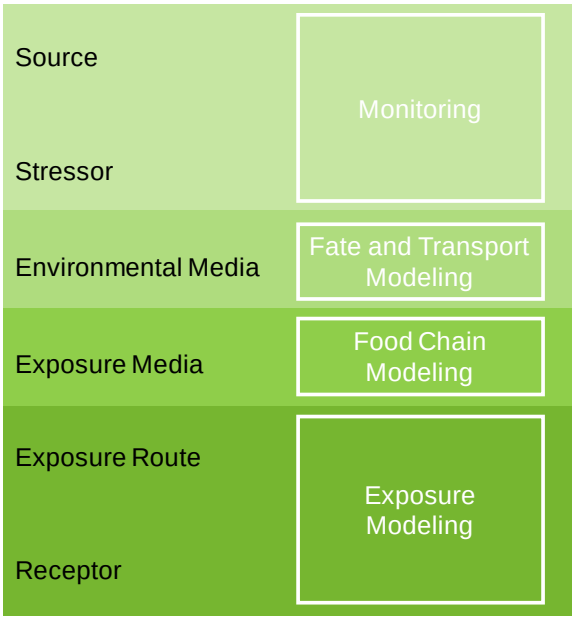
of the site so that we have a complete understanding of the source. After collecting this information about the location or site, we can develop the conceptual model of exposure. This course focuses primarily on site-specific analyses (or perhaps regionally-focused assessments) rather than national-scale analyses. However, many of these same monitoring design components would be applicable to monitoring at any scale.

An example of one approach to structuring a monitoring plan is incorporated into a template developed by EPA's Region 9, available online at http://ndep.nv.gov/bca/brownfield_qa_plan07.htm. This template includes both a sampling and an analysis plan by combining components of a Quality Assurance Project Plan (QAPP) and a Field Sampling Plan (FSP) to document a monitoring plan (NDEP, 2004).

Conceptual Model

After gathering information about site location and site history, we will hopefully have identified the potential sources of contamination, the potentially contaminated media, and the potential exposure pathways. We can combine all of this information into a conceptual model such as the one depicted in Figure 2, which will help guide the remainder of the assessment.

Figure 2. Components of a Sample Conceptual Model



In planning our assessment, we have to think about what modeling we might need to conduct later and what monitoring data will be required for use as inputs or parameters for our models. For example, if surface water is a key exposure pathway, we might want data on flow rates, chemical concentrations in water, and water characteristics like pH and levels of dissolved oxygen. We might monitor contaminants in the discharge to surface water and then model downstream concentrations to which people might be exposed (U.S. EPA, 1989).

Sample Size and Locations

Our primary concern in developing or evaluating a monitoring plan is to ensure that the data collected by the monitoring activity can be used effectively in a quantitative exposure assessment. With regard to sample size, we need to consider the number of areas to be sampled, the type of statistical analyses we plan to do, and the statistical performance needed, including variability, power, and certainty. We might have to refine the sample size due to practical concerns about time, money, the availability of equipment and personnel, and the accessibility of the site (U.S. EPA, 1989).

Sampling methods might be purposive, random, or systematic depending on the objectives and constraints (e.g., time, resources) of the assessment.

- **Purposive sampling** refers to the selection of sample locations for very specific reasons. The reasons might be quite different at different locations within the same study or site. For example, we might need to identify or evaluate known contamination hot spots, determine the geographic extent of

contamination, or characterize background. All of these data might be needed as part of the same monitoring study. Purposive sampling is often appropriate for screening analyses when we are trying to determine if a problem exists, because sample locations, timing, methods, and other aspects of the sampling can be biased toward the highest potential exposures.

- Either **random** or **systematic sampling** might give us more defensible and useful results, but these approaches usually cost more and take longer. These methods often are used if a representative data set is desired.

Types of Samples

Based on sources of contamination and potentially contaminated media, we need to determine the types of samples to collect. Which media should be sampled? How many samples from each medium should be collected? How should the samples be collected? Field screening analyses can be helpful in determining what kinds of samples we need to collect, when, and from where (U.S. EPA, 1989).

The type of medium from which samples are collected influences the sampling method, design, and timing. We can take either **grab samples** (to represent a single location) or **composite samples**. A single surface soil sample collected 6 inches below the surface is an example of a grab sample. A sample that is a well-mixed combination of many samples also taken from 6 inches below the surface, but randomly distributed across an area of several square meters, is an example of a composite sample. Composite samples can also account for temporal variations in concentrations by taking a long-term average. Composite samples for air are sometimes referred to as **continuous samples**. An example of a continuous air sample is an ambient air sample taken over a 24-hour period, which would take into account variations in pollutant levels that result from traffic patterns near a roadway, process start-up and shut-down emissions from a nearby factory, or other sources. Note that this approach, however, would not let us see the variations over time—it simply takes them into account in averaging the overall sample.

2.2 Other Considerations for a Sampling Strategy

We need to also consider time and meteorology when evaluating a monitoring plan. Changes in seasons or amounts of rainfall can affect environmental conditions and the chemical concentrations in media. However, we have to balance the desire to capture all possible geographic or site-specific variability with the time and money this might require. Daily sampling for an entire year might give us the best data, but we may not have a year to complete the assessment or the financial or personnel resources to get this done. Accessibility to the area might also be restricted, thereby limiting our ability to perform comprehensive monitoring.

We have to ask ourselves, “How much information is enough to adequately estimate exposure and risk?” The answer to this question depends on how much uncertainty and variability are acceptable, taking into account the purpose, scope, and other qualities of the assessment (U.S. EPA, 1989).

3. DATA EVALUATION

After we gather monitoring data for a site, we need to organize and evaluate the collected data and then determine what will be most useful for our quantitative exposure assessment. Based on the data, we can look to see how chemical concentrations or site characteristics change over time and across locations. This will help us determine which chemicals and locations to include in the exposure assessment and what data will be most useful. We can evaluate the data with respect to quantitation limits, data qualifiers, blanks, and background concentrations. From this evaluation, we will have a data set to support our exposure assessment. This section covers some of the aspects of data evaluation and quality assurance.

3.1 Quantitation and Detection Limits

When we start to evaluate our data, we need to know the quantitation limits and detection limits for each chemical, medium, and analysis method.

- The **quantitation limit** (QL) is the level at which the analytical laboratory is confident in quantifying the mass/concentration in a sample. In one sense, it is the level where a stated concentration can be "trusted." A QL might be adjusted based on how the sample is prepared. For example, was the sample diluted before analysis? What kind of matrix is the sample in? These matrices can change the level at which we can reliably and repeatedly quantify a concentration.
- The **detection limit** (DL) is the level above which a chemist can claim that the constituent was present. There are different types of detection limits that laboratories report. For example, the DL could be an instrument detection limit (IDL) or method detection limit (MDL). These represent the limits above the random noise from an instrument or method. A chemical might be detected at the detection limit but at a level too low to be quantified reliably.

If a compound is found below the quantitation limit, but above the detection limit, the analyst can confirm the compound is present, but not reliably report at what level. Such values are referred to as **trace**. Chemicals that are **nondetect** (ND) are not present or present below the detection limit (Armbruster and Pry, 2008; U.S. EPA, 1989).

Data Qualifiers

When we examine analytical results from environmental chemical monitoring, we might encounter data qualifiers associated with measured values. **Data qualifiers** are letters used to indicate the laboratory's findings for samples that could not be quantified.

As an example, Figure 3 displays sample data for concentrations of tetrachloroethene measured in groundwater at four hypothetical locations. The first and third samples for Site 1 include the data qualifier U. **U** is short for "undetected" and means that the sample was analyzed for the chemical, but that it was not detected. The numerical value next to the U is the detection limit.

Remember that the detection limit is the lowest value at which a laboratory can confirm the presence of a contaminant. Because detection limits sometimes can be high relative to health-based criteria, we cannot always assume a nondetect means the contaminant is not present at levels of potential concern. Data can also be reported as less than the detection limit. For example, for Site 2, sample 1 is reported as "less than 30," which means that the detection limit for this chemical is 30. "30U" or "less than 30" are equivalent ways to

Figure 3. Data Qualifiers for a Hypothetical Data Set

Tetrachloroethene Concentration (µg/L)				
	Sample 1	**Sample 2**	**Sample 3**	**Sample 4**
Site 1	**40U**	40	**30U**	20
Site 2	**<30**	45	**TR**	40
Site 3	**ND**	35	40	40
Site 4	50	**BDL**	50	**0**

#U → Undetected where the # value is the detection limit

<30 → Less than detection limit of 30

BDL → below detection limit

ND → Non-detect

BMDL → below minimum detection limit

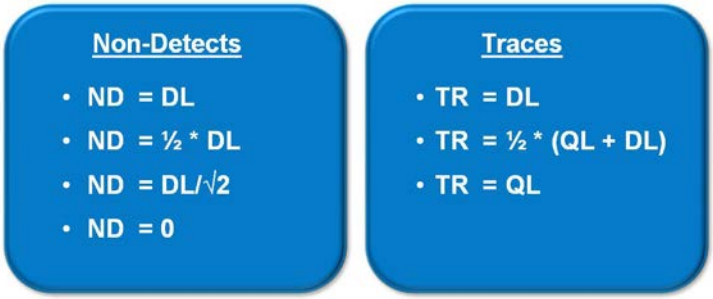
0 → ???

TR → Trace

present the same information. Other ways to indicate a nondetect include reporting values as **BDL** (below the detection limit), **BMDL** (below the minimum detection limit), or **ND** (nondetect). These reporting methods do not inherently provide the value of the detection limit. Notations of BDL, BMDL, or ND or measurements reported as "trace" are much more useful if accompanied by the value of the detection or quantitation limit.

Concentration values should not be reported as "0," as is shown for Site 4, Sample 4, in the example in Figure 3. Detection limits are nonzero values that need to be established by the laboratory conducting the analysis. A reporting of a "0" suggests a problem with the laboratory, or at least with the way they report measurements (U.S. EPA, 1991, 1989).

Treatment of Nondetects and Trace Measurements



In order for nondetects and trace-detects to be included in calculated statistics for use in exposure assessment, we can use different "substitution" methods. Nondetects can be set equal to the detection limit, half the detection limit, the detection limit divided by the square root of 2, or zero. Assessors often want to calculate averages for assumptions of both ND = 0 and ND = DL to demonstrate the impact of each of these approaches on results. When the overall average chemical concentration is very similar using both substitution methods, this demonstrates that the detection limits were sufficiently low for the data set being evaluated.

Trace detects are often set halfway between the quantitation and detection limits. Remember, a trace detect is one that is above the detection limit but below the quantitation limit. Measurements could also be set at either of these limits if so desired (U.S. EPA, 1991).

3.2 Background Concentrations

As discussed in EXA 404, "background" concentrations are those that occur from sources other than the source being evaluated, including both natural and anthropogenic sources. Background can mean the levels found in a regional area, but not attributable to a local source. These might include things such as background ozone

concentrations or chemicals from anthropogenic sources found in "pristine" areas. At some sites, contributions from background are significant and must be addressed.

Background must be somehow accounted for when the intent of the assessment is to characterize the contribution of a specific source. For example, chemicals found at CERCLA sites that are only attributable to naturally-occurring background concentrations are typically not included in cumulative risk calculations (U.S. EPA, 1992).

3.3 Assurance of Analytical Data Quality

Before we use monitoring data in an exposure assessment, it is important to make sure that the lab that produced the data is capable of accurately generating results—and that they implemented adequate quality assurance/quality control (QA/QC) procedures in the process. Quality control procedures can and should be implemented before (or independent of) a particular study, during the monitoring activities, and during analyses of study results.

A common pre-study procedure is a "demonstration of capabilities." In this procedure, a lab conducts analyses of a known chemical standard to make sure they have the technical ability to analyze for that chemical. Many chemical standards are available from the National Institute of Standards and Technology (NIST). As a part of this demonstration, the lab will compare its measurement results to the known concentrations in the standards to ensure that adequate mass recovery is accomplished—in other words, to make sure they are not "losing" mass of the analyte through the procedure.

Over the course of a study, a lab will typically incorporate other QC standards into the array of samples being evaluated for the study. Common standards include:

- Additional **chemical standards** containing known chemical concentrations to ensure the instruments are still operating as intended;
- **Duplicate samples**, which are identical samples that have been split into two to check the reproducibility of the data; and
- **Lab blanks**, which are samples free of the chemical of concern used to make sure no contamination was introduced from a nonsite-related source (e.g., during laboratory preparation or analysis).

Studies might also use a **recovery standard**. This standard contains a known concentration of a chemical added to a sample that is very similar to the chemical of concern, but not expected to be in the sample. A lab might use a radio-labeled standard to help determine if the chemical of interest is being lost or concentrated during the preparation or analytical process. This approach can help estimate the recovery of the analytes. Recovery standards are especially important when studying compounds that might volatilize from sampling matrices during the measurement process, thereby changing the measured concentrations of those compounds.

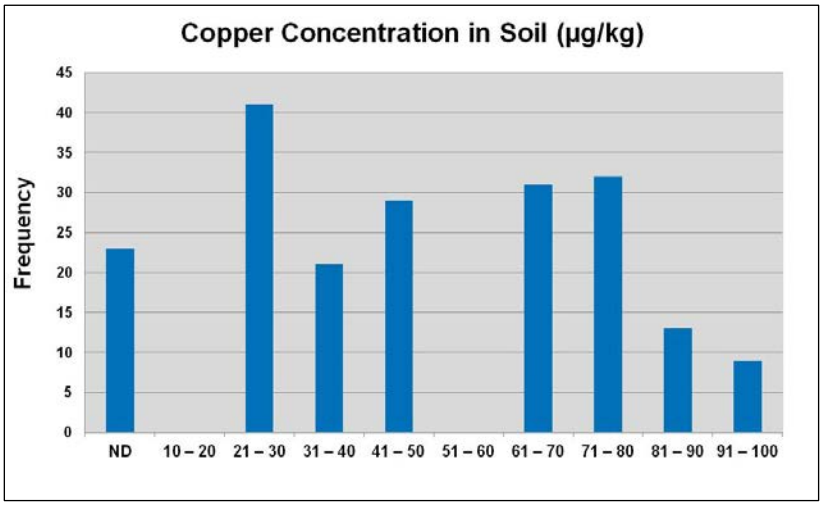
4. ASSEMBLING AND INTERPRETING DATA

This section discusses the review of data collected through monitoring. Different distributions can be useful in reviewing and interpreting data.

4.1 Frequency Distributions

A frequency distribution is a visual summary representation of monitoring data that presents the range of values obtained and the number of times, or frequency, that a given value (or set of values) was observed. Figure 4 presents a hypothetical frequency distribution depicting the range of concentrations of copper measured in soil in a monitoring study. Approximately 200 samples were collected, and sample results were grouped into nine concentration bins plus a tenth bin for nondetects. For example, as you can see in the figure, over 40 of the samples had concentration values between 21 and 30 µg/kg. This distribution shows that the copper soil concentrations at this site vary widely and do not exhibit a clear pattern. In order to better understand the true variability in soil copper concentrations at this particular site, it is likely that we would need to collect more samples. Some distribution shapes are observed frequently in environmental data sets; these are described below.

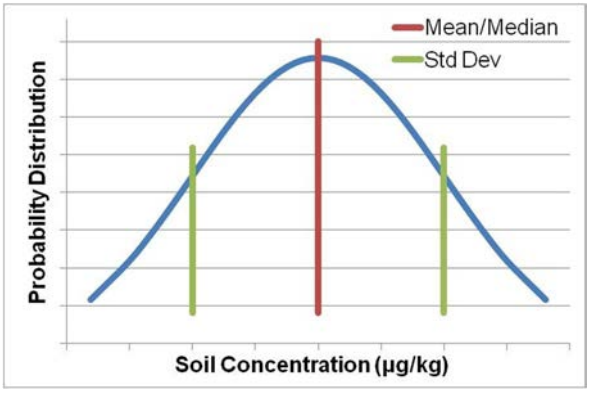
Figure 4. Sample Frequency Distribution



Normal Distribution

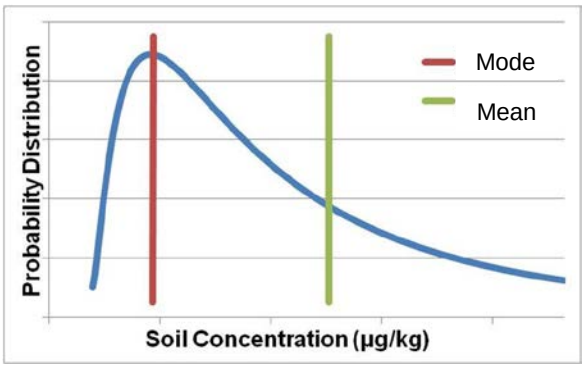
With a sufficiently large data set, values of some distributions of environmental parameters tend to take on a shape that is referred to as a **normal distribution**. A normal distribution, also called a Gaussian or bell-shaped curve, is one in which the mean, or average value, is the most common. As seen in Figure 5, the curve is symmetric about the mean, and the width of the curve is defined by the variance, or how much each value differs from the mean value. Generally, about 68% of the values in a normal distribution are within one standard deviation of the mean, and about 95% are within two standard deviations of the mean.

Figure 5. Example of a Normal Distribution



Lognormal Distribution

Figure 6. Example of a Lognormal Distribution

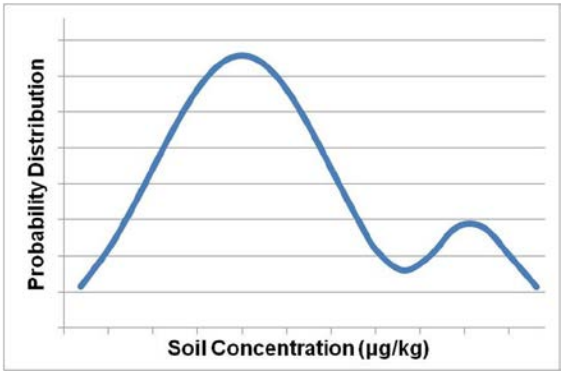


Many distributions of contaminants in environmental media are **lognormal** in distribution, like the data shown in Figure 6. These distributions often have values substantially larger than the mean or the median, resulting in a skewing of the distribution to the right. Lognormal distribution is the most common type of distribution for environmental and human exposure samples. If we transform the data by taking the log of each value, the resulting distribution is normal—a bell-shaped curve. Often a detection or quantitation limit is the lowest value on the x-axis of such a distribution. The right end of the tail is often what is of most interest.

Bimodal Distribution

A **bimodal distribution** is a more complicated frequency distribution that ones we have already discussed. A bimodal distribution has two maxima, or "humps," as shown in Figure 7. Bimodal distributions can result from a variety of circumstances. For example, it might occur if a particular variable or parameter changes with time or is affected by more than one source. It might occur if the source for measured concentrations has unusually large emissions on a periodic basis, such as during start-up or shut-down. Another example might be a distribution of exposures to a certain chemical present in both residential and occupational settings. The bump at the higher concentrations, further to the right end of the distribution and toward the tail, could represent the higher exposures for occupational settings. Bimodal distributions are more difficult to model, and they can require a higher number of samples to construct a representative distribution.

Figure 7. Example of a Bimodal Distribution



4.2 Data Interpretation

The "correct" sampling frequency and duration for a sample collection program might depend, in part, on whether the risk assessor is interested in measuring acute (short-term) or chronic (long-term) exposures. Likewise, the interpretation and use of the data collected depend on these temporal factors as well. If we are interested in acute exposures, a single point measurement might be adequate as long as the sample was collected at an appropriate point in time. However, in order to be more health protective, we might want to take many samples and use one with a high concentration. In this case, a frequency distribution can help you to determine how often exposures at that level might occur. If we are interested in chronic exposures, we will probably want to collect samples over a relatively long period of time. Then, the mean or median values in the middle of the resulting frequency distribution can help provide an estimate of an appropriate, representative

chronic exposure value to use. In addition, values from the upper end of the frequency distribution might help estimate the unlikely (but possible) upper bound of possible exposures (U.S. EPA, 1992).

5. MODELING EXPOSURE CONCENTRATIONS

Monitoring data can be used with environmental fate and transport models to better characterize media-specific exposure concentrations. When measured concentrations are not available, we can use models to estimate media concentrations and potential exposure concentrations in lieu of environmental data.

What is a Model?

Models can be thought of as a simplification of reality, analogous to a map. A map shows a part of reality to meet a specific purpose. Major roads would be shown on a driving map, but power lines would probably not be shown. Similarly, an environmental model shows or represents the part of the environment that is of interest and relevant, but it cannot show all processes that are occurring in the environment.

The National Research Council identifies five kinds of models that can help us understand physical and biological systems. A model can fit into more than one of these categories (NRC, 2007).

- **Physical:** A tangible representation of a more complex situation or system; for example, a solar system model using Styrofoam balls to represent the planets, moons, and sun
- **Analog:** Explains an event by reference to something else; for example, the use of mice and rats for toxicity testing based on the assumption that effects seen in these animals will be analogous to those seen in humans
- **Conceptual:** Illustration of the relationships between components (the relationships are not necessarily quantified)
- **Empirical:** An analytical approach that uses statistics to relate inputs to outputs
- **Computational:** The use of mathematical equations to predict real world happenings based on a series of equations, assumptions, and default parameters

Environmental Concentration Models

One of the most critical elements of a risk assessment is the estimation of pollutant concentrations at exposure points. For the remainder of this course, we are going to talk about environmental concentration models, but first, we will recap the two other kinds of models used in health risk assessment: exposure models and dose models.

Exposure models use mathematical relationships, ranging from simple static equations to complex, dynamic algorithms, to estimate exposure based in part on activities and physiological characteristics of the potentially exposed population. Exposure models can be used in conjunction with monitored or modeled environmental concentrations to better characterize exposure. Alternatively, in the absence of monitoring data to characterize exposure, models can be used to estimate exposure.

Dose models are another type of model used in risk assessment that estimate the amount of chemical in a tissue following exposure at the point of contact—in other words, the amount of chemical within the receptor domain half of the exposure to effects continuum presented in Figure 1. Of special interest to EPA are those that characterize internal dose, including physiologically-based pharmacokinetic models and benchmark dose models.

We use **environmental concentration models** to estimate chemical concentrations in environmental media, microenvironments, and surfaces. More specifically, environmental concentration models are used to model sources, emissions, and chemical transport and transformation—concepts covered in EXA 404—so that we can estimate the distribution of the chemical in the environment. This helps us to then estimate the concentration in the exposure medium or media to which our population of concern might be exposed.

The media included in an environmental concentration model can include air, water, soil, food or food webs, microenvironments, surfaces, biota, or a combination of any of these. Depending on the assessment, we can apply a modeling approach characterized as mechanistic or empirical, deterministic or stochastic, steady-state or dynamic, and screening-level or detailed—or sometimes a combination of some of these pairs. The fate and transport processes might be modeled based on first principles, partitioning, mixing, bioaccumulation, or a combination of these.

There are certain considerations that we have to be aware of when using models or model results in the context of risk assessment, especially critical assumptions underlying a modeling approach or application, the uncertainty associated with model results, and overall performance of the model. Ideally, modeling should be linked with monitoring data in regulatory assessments, although this is not always possible (e.g., for new chemicals, or when evaluating especially complex systems) (WHO, 2005; U.S. EPA, 1992).

5.1 Developing and Implementing an Environmental Modeling Strategy

Before using a model, we need to establish and put into action a modeling strategy. A good modeling strategy will specifically consider the objectives of the assessment to develop certain modeling objectives, and then will involve selection of a model that meets our objectives. It will also consider the appropriate level of evaluation, including calibration of the model for the specific assessment at hand (if required) and validation and verification the model's performance. Many of these aspects are analogous to the QA/QC procedures applied to measurements.

In the 1992 exposure guidelines, EPA highlights **validation** as an important part of the modeling process, with an emphasis on "ground-truthing" a model using measurement data. More recent publications, and in particular NRC's 2007 *Use of Models in Regulatory Decision-Making*, propose the use of the term **evaluation**. The rationale underlying this approach is that validation could be interpreted as a one-time activity intended to categorize models as "correct" or "incorrect." By using the term evaluation, the NRC and EPA recognize that there is a continuum of accuracy and usefulness. A model's characterization with respect to these attributes can be elucidated through a range of evaluations, including—but not limited to—comparison to measurements (NRC, 2007; U.S. EPA, 1992).

Setting Modeling Objectives

To begin, we must have clearly defined the goals of the exposure assessment. From there, we can determine what information a model or perhaps a combination of models will provide for the assessment at hand. We should also plan for how the model estimates will be used in the exposure assessment. Analogous to considerations for environmental monitoring, the approach we take for modeling should be consistent with the constraints of our project, including the schedule, budget, and other resources.

For example, a model could be used to calculate how a contaminant moves through the environment, such as from a stack to nearby surface waters. We could build this model equation by equation, or we could

parameterize an existing model that is designed to simulate similar environmental scenarios. How we choose to do this depends on our modeling objectives (U.S. EPA, 1992).

Model Selection

Selection of an appropriate model is not always a straightforward process. The International Programme on Chemical Safety of the World Health Organization (IPCS) directs us to consider six things when we select a model.

First, we need to consider the **mathematical** and **computational simplicity** of the model. Ideally, the model is only as complex as we need it to be and no more. More complexity does not necessarily mean better results. Sometimes increasing the complexity of a model can increase the uncertainty of the outputs without improving the accuracy or utility of the results. This idea is illustrated by the concept of Occam's razor, which is the principle that the theory that presents the fewest new assumptions is superior, if the only difference in the theories is complexity. It is also important to make sure that the results of the model we select can be **interpreted** (so that they are useful) and that they are **consistent** with our understanding of the science behind the process being modeled. It is also important that the results produced are consistent from site to site. A model that produces **accurate** results relies on inputs and equations that are valid. It is up to the assessor to ascertain the "accuracy" and "validity" of modeling outputs in the context of his or her assessment. Finally, it is important that the input values needed to run the model are **accessible**.

5.2 Model Evaluation

Principles of Model Evaluation

After selecting a model, we can evaluate how it suits the needs of our assessment. Evaluation should then continue through application and into the results processing stage. When we evaluate a model, we consider how well it represents the processes that are occurring in the environment and how well it helps us meet the goals of the analysis. A useful model might not always be the one that is the most realistic. Depending on the purpose of the model and the objectives of the assessment, a particular model might be adequate if you know that it is not underestimating concentrations. If it can be easily and quickly parameterized, a model might be preferable for reasons such as cost or a known pattern of historical use. Good screening models will strike an appropriate balance between accuracy and utility (Williams et al., 2010; NRC, 2007; U.S. EPA, 1992).

When using models for regulatory purposes, the National Research Council prescribes some questions to be considered(NRC, 2007).

- Does the model get the correct result within the context of the assessment? That is, does it have highly predictive powers?
- Does the model get the right result for the right reason? The model should be based on generally accepted science and computational methods, and the model should approximate the behavior of the system being modeled.
- Is the model transparent? The algorithms used by the model should be well documented, and the configuration and inputs used in that particular application. Additional complexity when it is not needed to adequately describe a process can introduce more uncertainty and make the model less transparent.

Methods for Evaluation

We can begin evaluating environmental concentration models by verifying that the transport and transformation concepts are appropriately represented in the mathematical equations. We can also verify that the model code is free of errors. For many of the environmental models used in applications for EPA, this will not be necessary if they have already been peer reviewed and documented.

One potentially straightforward way to evaluate a model's performance is to compare model outputs to measured values from field studies. In some cases, field data are specifically collected under controlled circumstances for purposes of model evaluation. Model results can also be compared to results from other models. Additionally, we can conduct evaluations using bounding or sensitivity analyses of the parameters used by the model. Bounding analyses allow us to evaluate how the model performs to achieve minimum and/or maximum results. Conducting a sensitivity analysis entails varying each parameter, either separately or together, to examine the impact of these parameter changes to model outputs.

The number of model evaluation steps that are performed is dependent on many factors and is the decision of the assessor. The extent of model evaluation will also depend on the certainty of the model and its inputs. The assessor might be limited by the amount of existing data that are available, as well as financial and time constraints (Williams et al., 2010; NRC, 2007; U.S. EPA, 1992).

6. MODEL CHARACTERISTICS

In this section, four approaches and frameworks for models are summarized, followed by descriptions of four types of environmental concentration models.

6.1 Modeling Frameworks

The first half of this section discusses four frameworks that can be used to classify modeling approaches. These classifications (which are not the only ways to classify models) are applicable to all types of models, not just environmental concentration or other exposure models.

Modeling Approaches Discussed Here:
Mechanistic vs. Empirical
Deterministic vs. Stochastic
Steady-State vs. Dynamic
Screening-Level vs. Detailed

Mechanistic Versus Empirical Models

Models can be mechanistic or empirical. The International Program on Chemical Safety (IPCS) of the World Health Organization defines **mechanistic models** as those that "simulate the real behavior of an agent in the environment and in target organisms as it is transported and undergoes physical and chemical transformations" [(WHO, 2005), page 15]. In mechanistic models, mathematical equations are used to connect physics, chemistry, and biology—processes we know happen in the real world—to predict concentrations based on our knowledge of the environmental fate and transport process. For example, in EXA 404, we talked about dispersion of chemical vapors or small particles in air, in which the ambient concentration patterns perpendicular to the wind direction follow a Gaussian distribution. This relationship has been applied to develop air quality dispersion models for air pollutants. When mechanistic models are developed, we do not necessarily need to have measurements (i.e., data) for both the inputs and the outputs in order to build the equations that connect them.

Empirical models are developed using data for both input and output variables and the relationships between model inputs and outputs. The IPCS definition specifies that "empirical models predict concentrations and exposures based on their statistical associations with concentrations in the relevant media and other independent variables that are observed in measurement studies" [(WHO, 2005), pages 15–16]. So, instead of expressing the relationship between these inputs and outputs with an equation based on physics, chemistry, or biology, empirical models use statistics and regression equations to link inputs to outputs. This means that empirical models cannot be built without measured data for both inputs and outputs. Thinking again to EXA 404, you may recall that we discussed bioconcentration and bioaccumulation factors for fish. These are based on measurements of chemicals in fish tissue and comparing them to chemical concentrations in the water. Applying a bioconcentration factor to estimate fish tissue concentrations is an example of an empirical model (WHO, 2005).

Deterministic Versus Stochastic Models

Models can be deterministic or stochastic, which are terms that refer to how model parameters or variables are set. **Deterministic models** use a single value for each input to produce a single value for each output. **Stochastic models**, on the other hand, can capture the variability in a data set because they can sample from a distribution of values for any (or all) of the parameters to produce a distribution of values for the outputs. Typically, these calculations cannot be completed by hand; stochastic models are typically more sophisticated and often rely on Monte Carlo simulations to predict outputs.

Another way to think about these two types of models is to consider deterministic models to be one run of a stochastic model. Remember that earlier we looked at normal, lognormal, and bimodal distributions of data. Stochastic models can incorporate the known or estimated variability in an input parameter because they are run over and over again using different input values, each selected from the input distribution to calculate the output values (WHO, 2005).

Steady-State Versus Dynamic Models

Similar to deterministic versus stochastic models, we can also classify models based on how (or if) the parameters change with time. **Steady-state environmental models** will have temporally constant values for all parameters, and chemical levels in each modeled compartment do not change over time. The chemical levels (or other predicted values) in such a model are at steady state. Running the model for additional time steps (that is, further into the future) will have no impact on modeled chemical concentrations. In a **dynamic model**, on the other hand, parameter values and the chemical concentrations being modeled can continue to change with time.

An advantage of steady-state models is that they tend to be quicker to run than dynamic models. However, for situations involving slow reactions (such as pollutants that are persistent in the environment or large aquatic systems that are slow to reach a steady state), a dynamic model might be more appropriate (WHO, 2005).

Screening-Level Versus Detailed Models

A primary consideration in selecting and applying a model is whether to perform a screening-level study or a more detailed evaluation. A **screening model** can be used to make a preliminary evaluation of an issue. A screening-level analysis is usually simple to perform and might be used to indicate whether or not a significant contamination problem exists. Often these models use very conservative assumptions; that is, they tend to overpredict concentrations or exposures, thereby sacrificing some accuracy in order to reduce uncertainty regarding whether a certain concentration or level of interest is reached or exceeded. Screening-level models are frequently used to get a first approximation of the concentrations that may be present. If the results of a conservative screening procedure indicate that predicted concentrations or exposures are much less than some predetermined no-concern level, then a more detailed analysis is probably not necessary. But, if the screening estimates are above that level, then refinement of the assumptions or application of a more sophisticated model might be necessary to get a more realistic estimate.

A more **detailed model** will be sophisticated and technically rigorous, and will usually involve more complex algorithms. Mechanistic and stochastic models are sometimes used instead of steady-state and/or empirical models when the data (and resources) are available for such a study. In reality, models tend to fall on a continuum from screening level to detailed. In addition, it is important to understand that the application of the model using specific parameters, and not just the model itself, determines if the modeled results are screening-level or more refined (U.S. EPA, 1992).

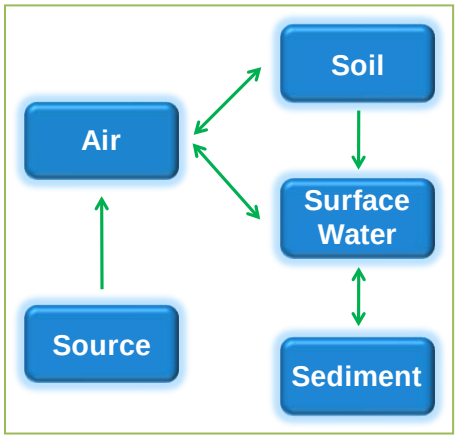
6.2 Types of Environmental Concentration Models

This section discusses four common types of environmental concentration models. The model constructs and approaches described here are, of course, not the only types of models, and it is common for a single model to incorporate two or more of the processes and principles described in this section.

First Principles

A model based on **first principles** is, essentially, a mechanistic model that translates scientific assumptions into a mathematical construct that can be used to predict behavior. An example is a fate and transport model that allows one to estimate the magnitude of chemical mass transfers between environmental media to obtain estimates of contaminant concentrations using principles of mass balance and transfer of mass between media. The simple conceptual model shown in Figure 8 depicts the possible chemical mass flow in a relatively simple version of such a model in which a single compartment is used to represent relevant types of environmental media. A mass-balanced model like this might apply the principles of fugacity to estimate chemical transfers between compartments (Mackay, 1991). Using this simple example, pollutant mass released from a source could be tracked as it deposits to soil or water (with some portion accumulating in sediments) and transfers between compartments, eventually reaching a steady state between sediment and surface water (U.S. EPA, 2005).

Figure 8. Conceptual Mass Flow Diagram of a First Principles Model



Partitioning

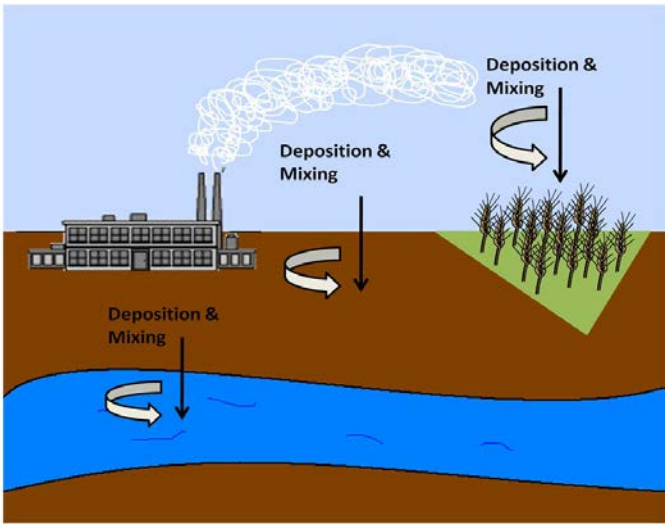
Partitioning models describe how contaminants move across the interfaces between media compartments in an environment, such as between water and air, water and soil, and water and biota. Remember from EXA 404 that the partition coefficient expresses the ratio of the chemical concentration in one environmental medium compared to the chemical concentration in another medium, with an interface situated between the two media. An example of this would be the partitioning between air and water for a volatile compound.

Modeling partitioning behaviors allows us to predict environmental concentrations in each compartment by applying principles of equilibrium. This is particularly useful when we are conducting screening-level approximations. Partitioning models by themselves do not capture transformation or other kinetic behaviors, but they can be combined with kinetic models to produce more detailed estimates. Dioxins, for example, are found sorbed to airborne particles, soils, and sediments and do not exist to any significant extent in the soluble or vapor phases, and therefore models developed for dioxins consider this partitioning behavior (McCall et al., 1983). The Mackay fugacity model referenced in the previous section on first principles models relies on fugacity concepts and notation to predict partitioning (Mackay, 1991). Note that is an example of a single model that falls into both of these categories.

Mixing Models

Mixing models are used to predict the concentration of a contaminant in a receiving environmental compartment as shown in Figure 9. These models describe the physical dilution of a contaminant in a medium of interest, such as soil or water. The chemical within a modeled compartment in a mixing model is often assumed to be homogeneously mixed throughout the compartment, and the mixing is assumed to occur instantaneously (i.e., immediately upon transfer of any mass into the compartment). These models can be very simplistic, but they also can be quite useful, especially for screening purposes.

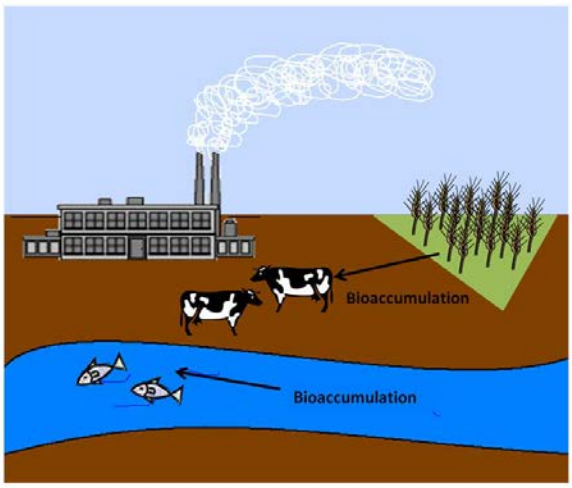
Figure 9. Examples of Simple Mixing Models

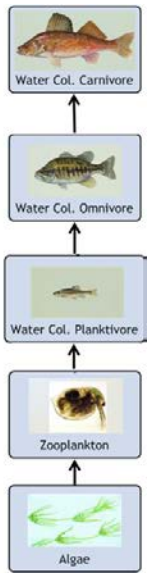


Bioaccumulation Models

Bioaccumulation models predict animal tissue concentrations as a simple linear product of food or media concentrations and a bioaccumulation factor, or BAF. As we discussed in EXA 404, bioaccumulation accounts for both direct uptake of a substance from an external medium (e.g., uptake from water through gills for a fish) and indirect food chain uptake (from ingestion of contaminated food). This is illustrated on the left side of Figure 10 where the bioaccumulation of a chemical in fish is being evaluated. Biotransfer, or BTF, models take a mass of contaminant in the feed of an animal (e.g., livestock) and convert it to a concentration in an animal product (e.g., beef, milk) (U.S. EPA, 2005, 2003).

Figure 10. Bioaccumulation Model





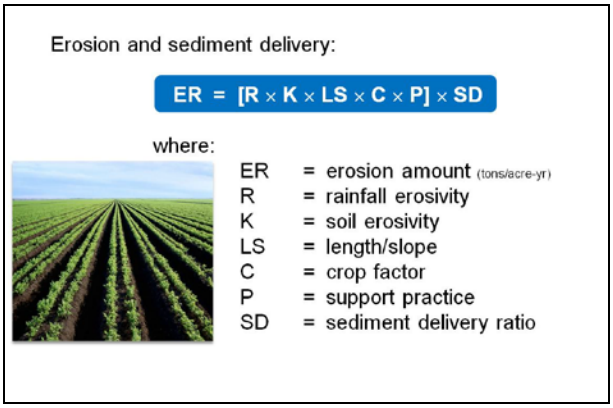
A bioenergetic model is a similar type of model that accounts for exchange of chemical mass between multiple levels of a food web. In the simplified fish food web depicted on the right side of Figure 10, the omnivorous and carnivorous fish accumulate more of the pollutant through their diet than planktivorous fish due to the transfer of chemicals up the food chain (i.e., through consumption of other contaminated animals), a process sometimes referred to as biomagnification. This has implications for humans who tend to eat fish that are higher in the food web (Arnot and Gobas, 2004).

7. EXAMPLES OF ENVIRONMENTAL CONCENTRATION MODELS

This section illustrates the concepts discussed previously in this course through three examples of specific environmental concentration models: the universal soil loss equation for modeling erosion; EPA's AERMOD air quality model; and PRAM and EXAMS, a pair of models used to assess exposures to pesticides. For a more comprehensive list of environmental models developed, used, or supported by EPA, the reader is referred to EPA's Models Knowledge Base compiled by the Council for Regulatory Environmental Modeling and posted online at http://www.epa.gov/crem/knowbase/index.htm.

7.1 USLE

Figure 11. USLE

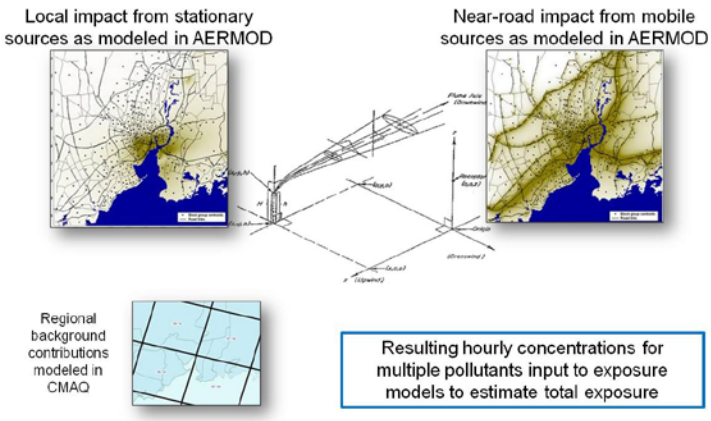


The **universal soil loss equation (USLE)** is a mathematical model for predicting soil erosion (see Figure 11). It was first circulated in 1940 as a method to predict erosion loss of soil from an agricultural field based largely on the length and slope of the field. Loss rates were based on erosion data obtained for farms in the Midwest and correlations developed between these erosion rates and field parameters; thus, it is an empirical model. The equation was further revised by adding additional factors to account for crops of varying types that can reduce erosion, conservation and other farming practices (like contour farming) that reduce erosion, and a rainfall factor based on the typical intensity and duration of rainstorms. In 1954, the equation and associated data tables were distributed by the National Runoff and Soil Loss Data Center, an extension of the Agricultural Research Service at that time. The supporting data for the equation have been expanded through the addition of other modifying factors, and lookups for some values have been automated via the internet. The sediment delivery ratio was also incorporated into the model. This is an empirical ratio that allows for the application of the USLE to large watersheds rather than the smaller farm plots for which the relationship was originally developed. Today, the modified version of the USLE is used in non-agricultural applications to estimate chemical transfers via erosive processes (Wischmeier and Smith, 1978).

7.2 AERMOD

The **AMS/EPA Regulatory Model (AERMOD)** estimates airborne concentrations at different point locations based on emissions of pollutants from a local source and the subsequent transport in the vicinity of the source via processes accounting for local meteorology. It is a steady-state, source-based Gaussian plume dispersion model typically used for chemically stable airborne pollutants. AERMOD is an example of a deterministic model.

Figure 12. Example of AERMOD Results

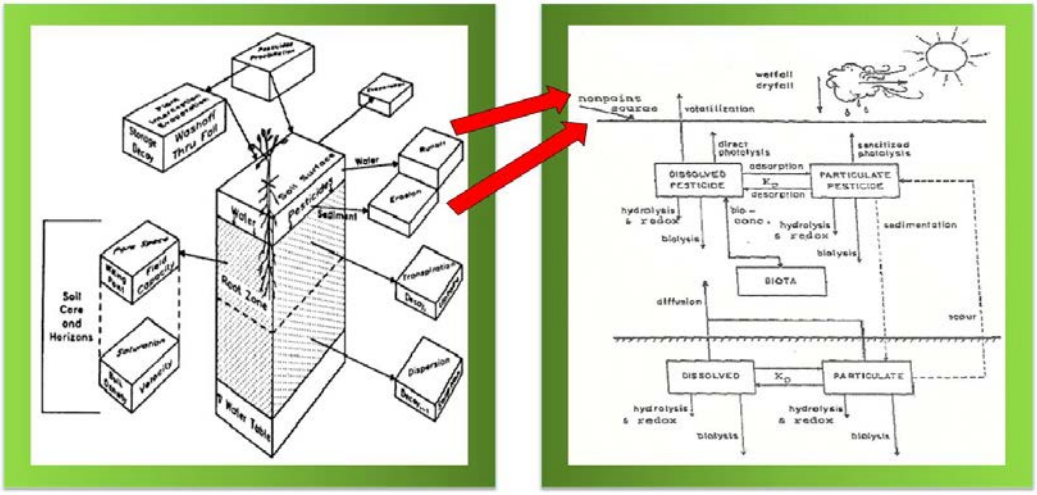


An example application of AERMOD, EPA's National Exposure Research Laboratory (NERL) has used this model to account (separately) for the contributions of stationary and mobile sources to the ambient concentrations in the New Haven, CT, metropolitan area, as depicted in Figure 12. In this analysis, NERL used a second model, the Community Multi-scale Air Quality (CMAQ) modeling system, to account for the chemistry and transport of pollutants from regional background contributions in this area. These three sets of concentration data were used in exposure models—HAPEM and SHEDS—to estimate total exposure concentrations for the people living in the New Haven area, with resolution retained to determine source contributions to the total exposure (Williams et al., 2010).

7.3 PRZM and EXAMS

The combination of **Pesticide Root Zone Model (PRZM)** and **Exposure Analysis Modeling System (EXAMS)** is a screening-level model used to estimate pesticide concentrations in water bodies for assessing human exposure to chemicals in drinking water sources and other aquatic exposures. These models are used by EPA's Office of Pesticide Programs (see Figure 13).

Figure 13. PRZM and EXAMS



The models are compartment or box models. Processes simulated in the model include application of a chemical or pesticide to a field, transport to a water body, chemical loading to a water body from other point and nonpoint sources, aerial drift of chemicals through the environment, washout of the chemical from the atmosphere, and groundwater seepage. PRZM has components that model pesticides through the root zone and into the groundwater, and also over the land surface. In this linked application, PRZM is used to estimate daily loads to a water body and EXAMS then estimates the water body concentrations. PRZM and EXAMS can be run either deterministically or stochastically to examine variability and uncertainty (Williams et al., 2010).

8. CONCLUSION

Both monitoring studies and modeling results can be valuable in conducting exposure assessments.

- Monitoring data provide direct measurements of the concentration of a contaminant in an environmental media, ideally at the point of contact for exposure.
- Monitoring data can be combined with modeling results to provide more information than the monitoring data provide alone.
- When monitoring data are unavailable because of cost, practicality, or other reasons, modeling might be the only way in which the concentration term can be estimated for an exposure assessment.

It is important when using either monitoring data or modeling results to ensure that data quality objectives have been met. When modeling, it is also important to select the appropriate model or combination of models to meet the exposure assessment objectives and to ensure that the appropriate level of model evaluation has been conducted.

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