EXA 405: Monitoring and Modeling Strategies
Instructor Notes

Course Description: 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 concepts (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 the discussion covering development and implementation of a modeling strategy, model types and limitations, and model evaluation. Several environmental models will be presented as examples.

Expected Course Duration: Approximately 1 hour

Terminal Learning Objective: Understand how monitoring data and modeling results are obtained, evaluated, and used in an exposure assessment.

Enabling Learning Objectives:

- Understand how a monitoring study is designed
- Understand how to interpret the quality of monitoring data, including censored data and background concentrations
- Understand the value and use of frequency distributions
- Understand why modeling is used in exposure assessment and how to apply a modeling strategy
- Develop a familiarity with types of models frequently used by EPA

Course Materials

- Reading Packet

Course Overview/List of Slides

TITLE SLIDE

- Welcome to EXA 405, on the fundamentals of environmental monitoring and modeling.

What You Can Expect to Learn from this Course (Slide 1)

- In the first part of this course, we'll introduce the basics of designing a monitoring study, collecting and evaluating data, and using these data in exposure assessments.
- We will discuss the metrics used to interpret data and evaluate data quality.
- Then we will talk about modeling environmental concentrations, including selecting an appropriate model, applying and using the model as part of our exposure assessment, and evaluating the model. We will discuss the types of environmental concentration models frequently used by EPA in risk assessment.
- The combined use of monitoring data and modeled results is a valuable approach for quantifying exposure for human health risk assessment.

Source to Effect Continuum (Slide 2)

- To picture where monitoring and modeling fit into exposure assessment, it's useful to refer again to the source to effect continuum we've introduced in previous courses. It's shown on this slide.
- 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. We're going to focus our discussion on the third part of the left side of the figure – that is, monitoring environmental concentrations to which people are exposed.
- The environmental models we will discuss in this course also inform components of the first half of source-to-effect continuum because they can account for pollutant fate and transport and model estimated environmental concentrations.
    - Other models can be used to model exposures, at the nexus of the two parts of the continuum (taking into account human behavior and time); we introduced some of these models in EXA 402. We won't cover those in this current course.
    - A third category includes models that estimate dose. We will not focus on those in this module, either.
- Let's begin by talking about environmental monitoring.
- Source: (Williams et al., 2010)

MONITORING STUDY DESIGN AND DATA GATHERING APPROACHES (SLIDE 3)

- There are many reasons for environmental monitoring of pollutants. In this course, we are going to focus on monitoring conducted to better understand human exposure. Specifically, we'll talk about monitoring of concentrations of chemicals in environmental media. We've discussed in other modules how we can monitor exposure concentrations

directly like through the use of personal exposure monitors, so we won't talk about that here.

Why Monitor? (Slide 4)

- Environmental monitoring provides the concentration term 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 may be potentially exposed.
- We begin monitoring by designing a study or sampling plan, or at the very least, we have to understand someone else's study design before using their data.
- Source: (U.S. EPA, 1989)

Study Design Considerations (Slide 5)

- There are some important considerations that we have to think through when designing or evaluating a study that involves monitoring data.
- The first is why is the study being conducted? What question is the study looking to answer?
- The second is 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 – that is, where the study begins and ends; and the timescale – that is, whether exposure is likely to be acute or chronic.
- The third question to ask is how accurate the measurements must be to meet the intended uses. How is the monitoring program limited by resources (time and money), and what is the most effective use of those resources to fulfill our goals? In other words, what is the appropriate level of detail?
- Finally, once the purpose, scope, and level of detail have been defined, we must determine how the concentrations in the media of interest will be measured – that is, our specific approach to measurement.
- So what goes into a monitoring plan? Let's talk about this.
- Source: (U.S. EPA, 1992)

Components of a Monitoring Plan (Slide 6)

- In designing a monitoring plan to support an exposure assessment, we need to consider information on the site, location, or scenario that might direct our data collection. Based on our knowledge of the scenario, 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 plan because it helps us to identify the potential contaminated media, determine how those chemicals are transported between media, and identify potential exposure routes. The site history will probably offer additional information that is important to our exposure assessment.
- If previous assessments have been conducted at a site or for the same exposure scenario, they could offer insight into the current assessment and also provide metrics for comparison. We need to also 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.
- Our discussion today is focused primarily on site-specific analyses (or perhaps regionally focused assessments) rather than on national-scale analyses. However, many of these same monitoring design components are applicable to monitoring for the National Air Toxics Assessment in the same way they're applicable to monitoring at an individual Superfund site or for a particular exposure scenario of interest (such as a specific occupational setting).
- Source: (NDEP, 2004)

Conceptual Model (Slide 7)

- After gathering information about the location we're assessing, we can identify the potential sources of contamination, the potentially contaminated media, and the potential exposure pathways. We can combine all of this information in a conceptual model which will help guide the remainder of the assessment.
- In planning our assessment, we have to think about what modeling we might need to do and what monitoring data will be required to 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, concentrations, and water characteristics like pH and dissolved oxygen. We might monitor contaminants in the discharge to surface water and then model downstream concentrations that people might be exposed to.
- Source: (U.S. EPA, 1989)

Sample Size and Locations (Slide 8)

- Our primary concern in developing or evaluating a monitoring plan is to ensure that the data collected by the monitoring activity can be used 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 with the data, and the statistical performance, 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 area.
- There are three ways we might determine sampling locations.
    - **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, to determine the geographic extent of contamination, or to characterize background – or determine all of these as part of the same monitoring study.
    - Purposive sampling is often most appropriate for screening analyses when we are trying to determine if a problem exists.
    - Either **random** or **systematic sampling** might give us more defensible and useful results – but these approaches usually cost more and take longer.
- Source: (U.S. EPA, 1989)

Types of Samples (Slide 9)

- Next we need to think about the types of samples to collect. From which media do we need to collect them? And the more difficult question, how should we collect them?
- The type of medium from which samples are collected influences the sampling method, design, and timing.
- We can take either grab samples or composite samples.
    - A single surface soil sample collected 6 inches below the surface is an example of a grab sample.
    - A sample that's 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 near a roadway, which would take into account variations in pollutant levels that result from traffic patterns, process start-up and shut-down emissions from a nearby factory, or other sources.
    - Note that this approach, though, wouldn't let us see the variations over time – it simply takes them into account in averaging the overall sample.
- Field screening analyses can help us determine what kinds of samples we need to collect, when, and from where.
- Source: (U.S. EPA, 1989)

Other Considerations for Sampling Strategy (Slide 10)

- 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. But we have to balance the need 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 the ability to monitor.

- 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 is acceptable, taking into account the purpose, scope, and other qualities of the assessment.
- Source: (U.S. EPA, 1989)

DATA EVALUATION (SLIDE 11)

- 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.

Data Evaluation Steps (Slide 12)

- After gathering all of 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 we'll use, among other things.
- Next we can evaluate the data with respect to quantitation limits, data qualifiers, blanks, and background concentrations.
- From this evaluation, we'll have a dataset to support our exposure assessment.
- Let's go over these steps.

Quantitation Limits (Slide 13)

- When we start to evaluate our data, we need to know the quantitation limits and detection limits for each chemical, medium, and analysis method.
    - [For instructor: Quantitation may sound like a made-up word, but it is referenced by EPA in the Risk Assessment Guidance for Superfund, or RAGS.]
- The **quantitation limit** or 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? Soil? Water? These matrices can change the level at which we can reliably and repeatedly quantify a concentration.
- The **detection limit** is the level, above which, a chemist can claim that the constituent was present. The detection limit is chemical, instrument, and method specific. It's the limit 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. We call these values "**trace**."
- **Nondetects** are exactly what you think they are: they are below the detection limit. We'll discuss how to deal with those in a bit.

- Sources: (Armbruster and Pry, 2008; U.S. EPA, 1989)

Data Qualifiers (Slide 14)

- When we examine analytical results for a chemical in a medium, we may encounter data qualifiers with the measured values. Data qualifiers are letters that indicate the laboratory's findings for samples that could not be quantified.
- Here on this slide we have 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.

? Why do you think the detection limit is different for the two samples?

  - Matrix interference is one possible reason; different matrix compositions could affect each measurement differently.

- 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 assume a non-detect 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" and "less than 30" are equivalent ways to present the same information.
- Other ways to indicate a non-detect include reporting values as
  - BDL, below the detection limit;
  - BMDL, below the minimum detection limit; or as
  - ND, a non-detect. These reporting methods do not provide the detection limit itself.
  - A notation of "below detection limits" or non-detect, or a measurement reported as "trace," is much more useful if it's accompanied by a detection or quantitation limit.
- Values should never be reported as zero. Detection limits are non-zero 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).
- Source: (U.S. EPA, 1991, 1989)

Treatment of Non-Detects and Trace Measurements (Slide 15)

- In order for non-detects and trace-detects to be included in calculated statistics for use in exposure assessment, we can use different "substitution" methods. Non-detects 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 display averages assuming ND = 0 and ND = DL to demonstrate the impact of the analytical method on results. When the average is very similar using both substitution methods, this demonstrates that the detection limits were sufficiently low for the dataset being evaluated.
- Trace detects are often set halfway between the quantitation and detection limits. Remember, a trace detect is one that's above the detection limit but below the quantitation limit. Measurements could also be set at either of these limits if so desired.
- Source: (U.S. EPA, 1991)

Treatment of Non-Detects and Traces – Class Activity (Slide 16)

- Let's do a class exercise to look at the impact of using the three substitution approaches for samples below the limit of detection. Here is the same sample table again, with reported tetrachloroethene concentrations measured in water samples.
    - As we mentioned a few slides ago, it's possible that there can be different detection limits for the same chemical in the same medium. In the example on this slide, the water samples may have had different characteristics even though they were taken from the same lake.
- For this exercise, I'd like you to calculate the range of overall average concentrations of tetrachloroethene in the lake we could get by using different assumptions. For non-detects, the measurements could be set to:
    - the detection limit,
    - half of the detection limit, or
    - to zero
- The measurements reported as trace could be set to:
    - the detection limit,
    - half of the sum of the detection limit and the quantitation limit, or
    - the quantitation limit.
- Why don't you take about 5 minutes to do this? The goal here is to calculate the extent of the range – in other words, the maximum and minimum of the calculated average that you might come up with.
    - Class may need guidance on identifying the minimum and maximum possible averages. There are lots of different possible "averages;" we are interested in getting just the lowest and the highest average.
    - Note that unless otherwise specified, the detection limit is 30 µg/L and the quantitation limit is 40 µg/L.
    - To calculate the maximum possible average, ND = DL and TL = QL.
    - To calculate the minimum possible average, ND = 0 and TL = DL.
    - Answers are on the following slide.

Treatment of Non-Detects and Traces – Results (Slide 17)

- (Give the class about 5 minutes to either calculate the averages or to estimate the magnitude of the differences between the averages calculated using the 3 substitution methods for non-detects and the 3 substitution methods for traces.)
    - (Click to bring up table of values. Slide appears with just the substitution method that yields maximum concentration first.)

? How did you find the highest, or maximum, possible average concentration?

- (Click to show ND = DL and TL = QL and average = 36.9.)
- (Click to remove table with maximum possible average; slide content will fade away.)
- (Click again to bring up table with values for minimum possible average calculation.)

? How about the lowest, or minimum, possible average concentration?

- (Click to show ND = 0 and TL = DL and average = 24.4.)

- The method used to evaluate non-detects and traces can have a significant impact on the reported concentrations. It's really important that we first report how we've treated the non-detects and traces and second consider what impact this might have on our results.

Background Concentrations (Slide 18)

- 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. At some sites, contributions from background are significant and must be addressed.
- Background can be defined as contributions of chemicals from natural sources (that is, not 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.
- Background must be somehow accounted for when the intent 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.
- In some cases, there is no specific "source" that has been identified or is being evaluated.

? Can you think of an example of a natural source of background chemical concentrations?

- Volcanoes, naturally occurring arsenic (e.g., in groundwater), naturally occurring metals that are present in soil

- Source: (U.S. EPA, 1992)

Assurance of Analytical Data Quality (Slide 19)

- Before we use monitoring data in an exposure assessment, it's important to make sure that the lab that produced the data is capable of accurately generating results – and that they implemented adequate QA/QC procedures in the process.
- Quality control procedures can and should be implemented before (or independent of) a particular study as well during analyses and as part of a study.
- A common pre-study procedure is a "demonstration of capabilities." This is where 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 or 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 with 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 other contamination has occurred.
    - Recovery standards with known chemical concentrations, to determine if the chemical of concern is being lost or concentrated during the preparation of analytical process.

ASSEMBLING AND INTERPRETING DATA (SLIDE 20)

- Now we will shift gears and talk about using data collected through monitoring. We'll talk about how frequency distributions can be useful in reviewing and interpreting data.

Frequency Distribution (Slide 21)

- A frequency distribution is a visual 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.
- Presented here is a frequency distribution depicting the range of concentrations of copper that was measured in soil in a monitoring study. The frequency, or number of times each concentration was measured, is shown for about 200 samples, with observations binned into nine concentration bins, plus a tenth bin for non-detects.
    - For example, about 40 of the samples had a value of between 21 and 30 µg/kg, and about 10 of the samples had a concentration of between 91 and 100 µg/kg.

- This distribution shows that the copper soil concentrations at this site vary widely and without a clear pattern; the frequency distribution of the data is quite random.
- In order to understand the true variability in soil copper concentrations at this particular site, it's likely that we would need to collect more samples.

Normal Distribution (Slide 22)

- With enough measurements, values of some distributions of environmental parameters can take on a shape that's 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. 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.

Lognormal Distribution (Slide 23)

- Many distributions of contaminants in the environment and exposure media are lognormal in distribution, like the data shown in this figure. 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.
- Let's talk about one more type of distribution that we might encounter.

Bimodal Distribution (Slide 24)

- There are more complicated frequency distributions that you might see. One is a bimodal distribution, which has two maxima, or "humps."
- Bimodal distributions can result from any number of circumstances, such as a variable or parameter that changes with time or is affected by more than one source. Or, the source for the measured concentration periodically has unusually large emissions 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 – that is, further to the right end of the distribution and toward the tail – could represent the higher exposures for occupational settings.

- These distributions are more difficult to model, and they can require a higher number of samples to construct a representative distribution.

Data Interpretation (Slide 25)

- The "right" sampling frequency and duration of the sample collection program 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 as well.
- If we're interested in acute exposures, a single point measurement might be adequate, as long as it was collected at an appropriate point in time.
    - However, in order to be more health-protective, we might want to take a lot of samples and use one with a high concentration. In this case, a frequency distribution can help you to determine how often exposures at that magnitude might occur.
- If we're interested in chronic exposures, we'll 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 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.
- Source: (U.S. EPA, 1992)

MODELING EXPOSURE CONCENTRATIONS (SLIDE 26)

- Monitoring data can be used with environmental fate and transport models, to better characterize exposure media concentrations.
- Or, when measured concentrations are not available at all, we can use models to estimate environmental and exposure concentrations.

What is a Model? (Slide 27)

- The National Research Council identified the five kinds of models listed on this slide that help us "gain insights" into physical and biological systems. A model can fit into more than one of these categories.
- A simple example of a physical model, something you can touch, could be created using Styrofoam balls to represent the planets, moons, and sun in our solar system. A slightly different kind of example that we are all familiar with is the use of mice and rats for toxicity testing. This model is based on the assumption that effects seen in these animals will be analogous to those in humans.
- Conceptual models show the relationships between components, but these relationships aren't necessarily quantified. Empirical models use statistics to relate inputs to outputs. We'll talk more about these in a minute.

- Finally, computational models use mathematical equations to predict real world happenings based on a series of equations, assumptions, and default parameters. We'll focus primarily on computational models for the remainder of the course.
- Source: (NRC, 2007)

Why Model? (Slide 28)

- 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, but it cannot show all processes that are occurring in the environment.
- 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're going to talk about environmental concentration models, but first, let's recap the two other kinds of models used in health risk assessment.
- **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. Or, 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. Of special interest to us are those that characterize internal dose like physiologically-based pharmacokinetic models and benchmark dose models.
- For all three of these kinds of estimates, there are certain considerations that we have to be aware of when using models or model results. For example, EPA's Science Advisory Board has concluded that, ideally, modeling should be linked with monitoring data in regulatory assessments, although this is not always possible (e.g., for new chemicals). We will talk about other considerations too.
- Sources: (WHO, 2005; U.S. EPA, 1992)

Environmental Concentration Models (Slide 29)

- Let's talk specifically now about environmental concentration models.
- We use these 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 that our population of concern might be exposed to.

- Depending on the assessment, we'll 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, or bioaccumulation, or a combination of these.
- And the media modeled might be air, water, soil, food or food webs, microenvironments, surfaces, or a combination of any of these.
- We'll talk about these modeling approaches and processes in a bit.

IMPLEMENTING AN ENVIRONMENTAL MODELING STRATEGY (SLIDE 30)

- But first, let's look at the bigger picture. Before using a model, we need to establish and put into action a modeling strategy.

Implementing a Modeling Strategy (Slide 31)

- A good modeling strategy will specifically consider the objectives of the assessment to develop certain modeling objectives, and then involve selection of a model that meets our objectives. Next, we must calibrate the model (if that's required) and validate and verify the model's performance. Many of these aspects are analogous to the QA/QC procedures applied to measurements.
- Let's quickly review the use of the terms validation and evaluation.
    - In the 1992 exposure guidelines, EPA lists 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" on the grounds that validation could be interpreted as a one-time activity, and based on the idea that models cannot be validated as "correct" or "incorrect." Instead, there is a continuum of accuracy and usefulness, and 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.
- Source: (NRC, 2007; U.S. EPA, 1992)

Setting Modeling Objectives (Slide 32)

- To begin, we must have clearly defined the goals of the exposure assessment. From there, we can determine what information a model or maybe a combination of models will help estimate. We should also plan for how the model estimates will be used in the exposure assessment. Just as with 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's designed to simulate similar environmental scenarios. How we chose to do this depends on our modeling objectives.

- Source: (U.S. EPA, 1992)

Model Selection (Slide 33)

- Selection of an appropriate model might not be a straightforward process. The IPCS (International Programme on Chemical Safety of the World Health Organization) 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 complex doesn't necessarily mean better results. Sometimes increasing the complexity of a model just increases the uncertainty of the outputs.
    - This idea is illustrated by the concept of Occam's razor. This is the principle that the theory that presents the fewest new assumptions is superior, if the only difference in the theories is complexity.
- It's also important to make sure that the results of the model can be **interpreted** and that they are **consistent** with our understanding of the science behind the process being modeled but also that the results produced are consistent from site to site.
- A model that produces "**accurate**" results relies on inputs and equations that are valid. "Accurate" is a subjective term of art in this context – it is up to the assessor to ascertain the "accuracy" and/or "validity" of modeling outputs in the context of his/her assessment.
- And finally, it's important that the input values needed to run the model are accessible.
- Once we have selected a model, gathered the required input values, and run the model, we need to evaluate the results.
- Source: (WHO, 2005)

Principles of Model Evaluation (Slide 34)

- After selecting a model, we'll evaluate how it suits the needs of our assessment. Evaluation then continues 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.
    - A useful model might not always be the one that's the most realistic. Depending on the purpose of the model and the objectives of the assessment, one model might be adequate if you know that it is not underestimating concentrations and can be easily parameterized, and this model might be preferable for reasons such as cost or a known pattern of historical use. Good screening models will appropriately strike a balance between accuracy and utility.
- When using models for regulatory purposes, the National Research Council prescribes some questions to be considered.

    - The first question is: does the model get the correct result? That is, does it have highly predictive powers?
    - Secondly, 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.
    - The final question is: Is the model transparent? The algorithms and inputs used by the model should be well-documented. Additional complexity when it's not needed to adequately describe a process can introduce more uncertainty and make the model less transparent.
- Source: (Williams et al., 2010; NRC, 2007; U.S. EPA, 1992)

Methods for Evaluation (Slide 35)

- Here are a few of the methods for evaluating environmental concentration models.
- We can begin 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 models that we'll use, this will not be necessary because they will have already been peer reviewed.
- We can 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.
- The model results can also be compared to results from other models.
- Finally we can conduct evaluations with sensitivity or bounding analyses. Bounding analyses allow us to evaluate how the model performs to achieve minimum and/or maximum results. Conducting a sensitivity analysis, on the other hand, entails varying each parameter, sometimes separately and sometimes together, to examine the impact of these parameter changes to model outputs.
- Source: (Williams et al., 2010; NRC, 2007; U.S. EPA, 1992)

MODELING APPROACHES (SLIDE 36)

- Let's continue our discussion by talking about four ways to classify modeling approaches. These classifications are applicable to all types of models, not just environmental concentration or other exposure models. You might recall that we briefly touched on these at the beginning of our discussion of models.

Mechanistic Versus Empirical Models (Slide 37)

- First, models can be mechanistic or empirical. The definition here of mechanistic models comes from the International Program on Chemical Safety and says, "mechanistic models 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.
- The inputs for mechanistic models can be single values, point estimates, and the outputs are then point estimates. When mechanistic models are developed, we do not have to have measured data for both the inputs and the outputs in order to build the equations to connect them.
- This is different from empirical models. Empirical models are developed based on measurement data of input and output variables, and the relationships between inputs and outputs.
    - The IPCS definition says 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 concentrations in the water. Applying a bioconcentration factor to estimate fish tissue concentrations is an example of an empirical model.

Source: (WHO, 2005)

Deterministic Versus Stochastic Models (Slide 38)

- 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 natural variability in a dataset 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.
    - Obviously, we cannot do this math with just a calculator; stochastic models are more sophisticated and often rely on Monte Carlo simulations to predict outputs.
- Another way to think about these two types of models 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.

Source: (WHO, 2005)

Steady-State Versus Dynamic Models (Slide 39)

- 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 will not change over time.
    - The chemical levels (or other predicted values) in such a model have reached 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 long-lived in the environment, or large aquatic systems that are slow to reach a steady state), a dynamic model might be more appropriate.

Source: (WHO, 2005)

Screening-Level Versus Detailed Models (Slide 40)

- A final characterization of models is as a screening-level or detailed model.
- A primary consideration in selecting a model is whether to perform a screening 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 may indicate that no significant contamination problem exists. Often these models use very conservative assumptions; that is, they tend to over-predict concentrations or exposures.
- 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 need and 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, 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.
- Source: (U.S. EPA, 1992)

TYPES OF ENVIRONMENTAL CONCENTRATION MODELS (SLIDE 41)

- Let's talk more specifically now about environmental concentration models.

First Principles (Slide 42)

- A first principles model is one that estimates environmental concentrations based on established scientific principles, such as known chemical, physical, and biological relationships. As such, it is a type of mechanistic model.
- This simple conceptual model depicts the chemical movement that could be simulated in a fate and transport model. We often illustrate the concepts of a model using block diagrams like this one to show the "physical, chemical and behavioral information and exposure algorithms" used in the model to mathematically express the exposure scenario [(WHO, 2005); page 12].
- Fate and transport models are used to predict the movement of contaminants between and within compartments
- On this slide, a pollutant released from a source could be moved by the wind, deposited to soil or water, and transferred between each of these compartments, eventually reaching a steady state between sediment and surface water.
- A fate and transport model would allow you to estimate the magnitude of these transfers to get to contaminant concentrations in the media of interest.
- Source: (U.S. EPA, 2005)

Partitioning (Slide 43)

- Partitioning models describe how contaminants "partition" 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. An example of this would be the partitioning between air and water for a volatile compound.
- Modeling these partitioning behaviors allows us to predict environmental concentrations in each compartment. 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. A partitioning model for dioxin would have to take this into account.
- Source: (McCall et al., 1983)

Mixing Models (Slide 44)

- Mixing models are used to predict the concentration of a contaminant in a receiving environmental compartment.

- 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 is often assumed to be homogeneously mixed throughout the compartment.
- These models can be very simplistic – but they can be quite useful, especially for screening purposes.

Bioaccumulation Models (Slide 45)

- Bioaccumulation models predict animal 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 from an external medium and ingestion of a substance. This is illustrated in the figure on the left side of the slide where the bioaccumulation of a chemical in cattle or fish is estimated.
- Biotransfer, or BTF, models take a mass of contaminant in the food intake of an animal and convert it to a concentration, for example in beef or milk.
- Source: (U.S. EPA, 2005, 2003)
- Similar types of models that account for exchange of chemical mass between multiple levels of a food web are termed bioenergetic models.
    - In the simplified fish pathway shown here on the right side of the slide, the omnivorous and carnivorous fish accumulate more of the pollutant through their diet than planktivorous fish due to the bioconcentration of pollutants into animals throughout the food web, and also the transfer of chemical up the food web through consumption of other, contaminated animals.
    - This has implications for humans who tend to eat fish that are higher in the food web.
- Source: (Arnot and Gobas, 2004)

EXAMPLE ENVIRONMENTAL CONCENTRATION MODELS (SLIDE 46)

- Let's go over a few examples of environmental concentration models.

Universal Soil Loss Equation (USLE) (Slide 47)

- The first one we'll talk about is the universal soil loss equation, or USLE, that can be used to predict erosion.
- A mathematical model for predicting erosion was first circulated in 1940; it predicted erosion loss based on the length and slope of a field and the prediction was based on measured data from farms in the Midwest. Thus, it's an empirical model.
- The equation was further revised by adding factors to account for the impact on erosion of growing certain crops, conservation and other farming practices that reduce erosion like contour farming, and a rainfall factor based on the typical intensity and duration of rainstorms.

    - In this equation, the R and K parameters represent how much erosion would occur from a "standard" plot of the soil of interest.
    - The LS, or length/slope factor, then adjusts the estimated erosion value by the steepness and length of the slope of the plot of interest, relative to a "standard" plot.
    - The C, P, and SD parameters are all unitless factors that adjust the estimated erosion rate to account for site-specific characteristics.
- In 1954, the equation and associated data tables were first widely distributed by the National Runoff and Soil Loss Data Center. The supporting data for the equation has been expanded (Revised Universal Soil Loss Equation [RUSLE]) and the lookup for some values automated via the internet. The sediment delivery ratio 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. The sediment delivery ratio will always be less than or equal to one and is multiplied by the product of the rainfall erosivity, soil erosivity, length/slope, crop factor, and support practice to predict how much soil gets to the area of concern.
- Source: (Wischmeier and Smith, 1978)

AMS/EPA Regulatory Model (AERMOD) (Slide 48)

- The second example is the American Meteorological Society (AMS) and U.S. Environmental Protection Agency (EPA) Regulatory Model, or AERMOD.
- AERMOD estimates airborne concentrations at different point locations based on emission and transport of pollutants emitted from a local source. It is a steady-state Gaussian plume dispersion model (i.e., source-based dispersion model) typically used for chemically stable airborne pollutants.
- AERMOD is an example of a deterministic model, because it uses a single value for each input to produce a single value for each output.
- Shown on this slide is EPA's National Exposure Research Laboratory or NERL use of AERMOD to model contributions of stationary sources like industrial facilities and mobile sources on roadways. The estimated concentrations of multiple pollutants in the New Haven, CT area are shown in the top two images on this slide. NERL also used CMAQ to model the chemistry and transport of pollutants from regional sources. These three sets of concentration data were used in exposure models – HAPEM and SHEDS – to estimate exposure concentrations for the people living in the New Haven area.
- Source: (Williams et al., 2010)

Pesticide Root Zone Model (PRZM) and Exposure Analysis Modeling System (EXAMS) (Slide 49)

- Finally, we'll introduce the combination of the Pesticide Root Zone Model, or PRZM, and the Exposure Analysis Modeling System, or EXAMS.

- This is a **screening-level model** used to estimate pesticide concentrations in water bodies to assess exposure to chemicals from drinking water or other aquatic exposure to chemicals. These models are used by EPA's Office of Pesticide Programs.
- The models are compartment or box models. Processes simulated in the model include
    - transport of a chemical or pesticide applied to a field to a water body,
    - chemical loading to a water body from point and non-point sources,
    - aerial drift of chemicals through the environment,
    - washout of the chemical from the atmosphere, and
    - groundwater seepage.
- PRZM has components that model movement of pesticides through the root zone and into the ground water, 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.
- Source: (Williams et al., 2010)

CONCLUSION (SLIDE 50)

- Let's wrap up with some conclusions.

Conclusion (Slide 51)

- Both monitoring studies and modeling results are 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 models to provide more information than monitoring data could provide alone.
- When monitoring data are unavailable (cost, practicality, and so on), modeling may be the only way in which the concentration term can be ascertained in an exposure assessment.
- It is important when using either monitoring data or modeling results to ensure that data quality objectives have been met, and that the model has been evaluated as thoroughly as possible.

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