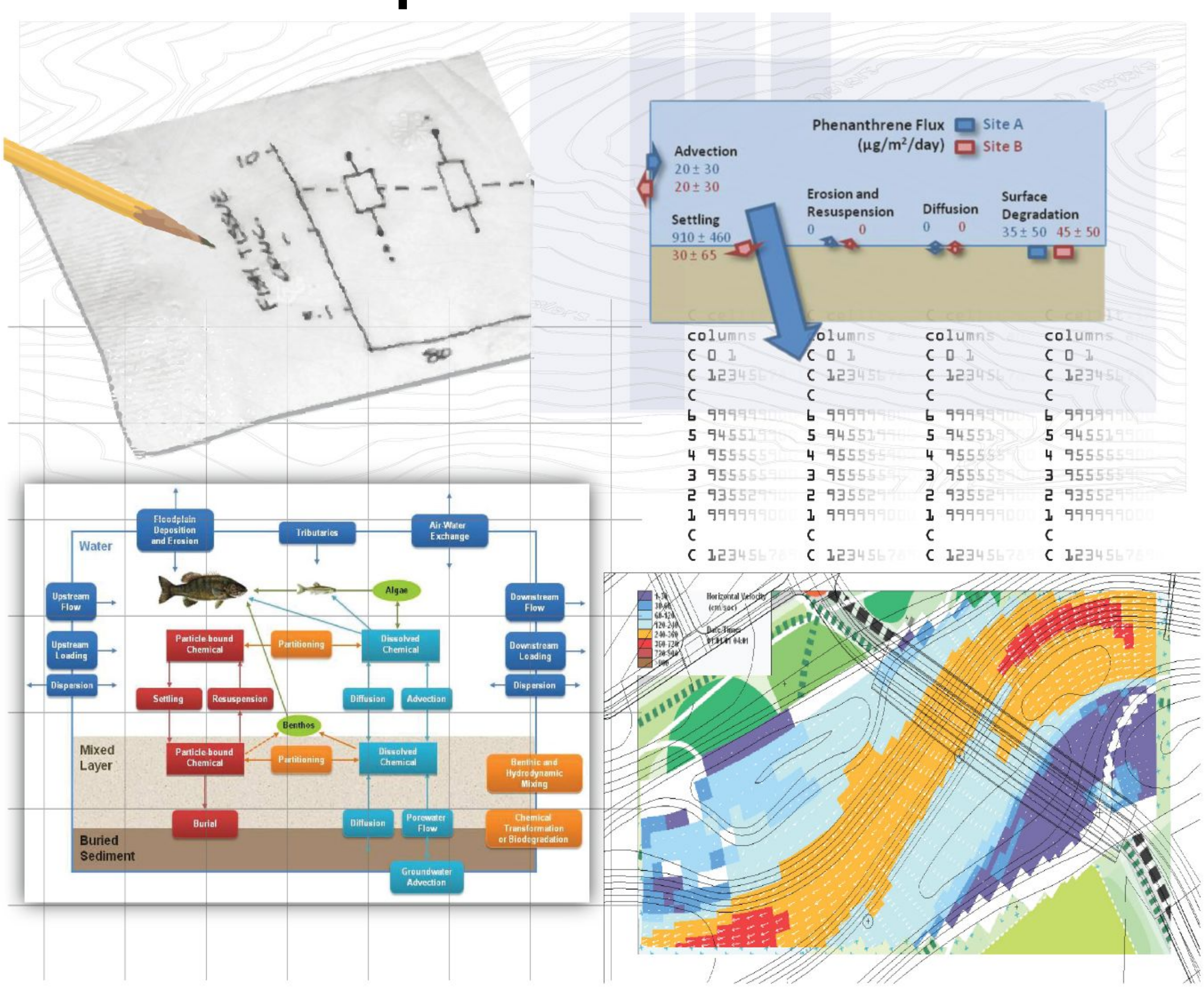
Office of Superfund Remediation and Technology Innovation

Sediment Assessment and Monitoring Sheet (SAMS) #2

Understanding the Use of Models in Predicting the Effectiveness of Proposed Remedial Actions at Superfund Sediment Sites



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SEDIMENT ASSESSMENT AND MONITORING SHEET #2

Background and Purpose

This is the second fact sheet in the Sediment Assessment and Monitoring Sheet (SAMS) series prepared by the Office of Superfund Remediation and Technology Innovation (OSRTI).

This product is a primer for those not experienced in the development and use of models at sediment sites. It explains the typical objectives of modeling, how models are built, how they are used to predict the effectiveness of remedies, and how the uncertainty in model predictions can be addressed. The document is not intended to provide site-specific direction on the application or data requirements of specific models.

This document does not supersede the guidance on modeling provided in section 2.9 of the 2005 Contaminated Sediment Remediation Guidance for Hazardous Waste Sites. That document provides guidance on determining whether mathematical modeling is needed and what level of modeling is most appropriate for a site, and discusses the need to verify, calibrate, validate, and peer-review models.

This document does not impose legally-binding requirements on EPA, states, or the regulated community, but suggests modeling approaches that may be used at particular sites, as appropriate, given site-specific circumstances.

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INTRODUCTION

Remedy evaluation at Superfund sites typically includes predictions of risk reduction for each potential remedial alternative. As discussed in the 2005 Contaminated Sediment Remediation Guidance for Hazardous Waste Sites (USEPA, 2005), "Models are tools that are used at many sediment sites when characterizing site conditions, assessing risks, and/or evaluating remedial alternatives. A complex computer model (e.g. multidimensional numerical model) may not be needed if there is sufficient weight of evidence distinguishing the best remedial option based on an adequate understanding of site conditions; however, this is not often the case. At some sites, significant uncertainties exist about site characterization data and the processes that contribute to relative effectiveness of available remedial alternatives. Models can help fill in gaps in knowledge and allow investigation of relationships and processes at a site that are not fully understood. For this reason, simple or complex modeling can play a role at most sediment sites." "Whether and when to use a model, and what models to use, are site-specific decisions and modeling experts should be consulted." http://www.epa.gov/superfund/health/conmedia/sediment/guidance.htm

This fact sheet is an introductory primer for managers of contaminated sediment sites who are seeking to better understand the purpose and appropriate use of environmental models. It explains how sediment models are built, calibrated, and used to make predictions of remedial outcomes, how to decide how much complexity to include, and also how to interpret predictions in the light of uncertainties and other limitations of data and modeling. Specifics regarding the development of data sets to support modeling, selection of environmental models, or site-specific application are not discussed in this document. The following sections of this Fact Sheet address these questions about models and their uses:

- What is Modeling?
- What's in a Model?
- What's Needed for a Model?
- How Certain are Model Predictions?
- How Do We Predict Remedial Outcomes?

Important Principles to Consider in Developing and Using Models at Sediment Sites (USEPA, 2005)

1. **Consider site complexity before deciding whether and how to apply a mathematical model.** Site complexity and controversy, available resources, project schedule, and the level of uncertainty in model predictions that is acceptable, are generally the critical factors in determining the applicability and complexity of a mathematical model. Potential remedy costs and magnitude of risk are generally less important, but they can significantly affect the level of uncertainty that is acceptable.
2. **Develop and refine a conceptual site model that identifies the key areas of uncertainty where modeling information may be needed.** When evaluating if a model is needed and in deciding which models might be appropriate, a conceptual site model should be developed that identifies the key exposure pathways, the key sediment and water-body characteristics, and the major sources of uncertainty that may affect the effectiveness of potential remedial alternatives (*e.g.* capping, dredging, and/or monitored natural recovery (MNR)).
3. **Determine what model output data are needed to facilitate decision making.** As part of problem formulation, the project manager should consider the following: 1) what site-specific information is needed to make the most appropriate remedy decision (e. g. degree of risk reduction that can be achieved, correlation between sediment cleanup levels and protective fish tissue levels, time to achieve risk reduction levels, degree of short-term risk); 2) what model(s) are capable of generating this information; and 3) how the model results can be used to help make these decisions. Site-specific data collection should concentrate on input parameters that will have the most influence on model outcomes.
4. **Understand and explain model uncertainty.** The model assumptions, limitations, and the results of the sensitivity and uncertainty analyses should be clearly presented to decision makers and should be clearly explained in decision documents such as proposed plans and records of decision (RODs).
5. **Conduct a complete modeling study.** If an intermediate or advanced level model is used in decision making, the following components should be included in every modeling effort:
    - Model verification (or peer-review if a new model is used)
    - Model calibration
    - Model validation
6. **Consider modeling results in conjunction with empirical data to inform site decision making.** Mathematical models are useful tools that, in conjunction with site environmental measurements, can be used to characterize current site conditions, predict future conditions and risks, and evaluate the effectiveness of remedial alternatives in reducing risk. Modeling results should generally not be relied upon exclusively as the basis for cleanup decisions.
7. **Learn from modeling efforts.** If post-remedy monitoring data demonstrate that the remedy is not performing as expected (*e.g.,* fish tissue levels are much higher than predicted), consider sharing these data with the modeling team to allow them to perform a post-remedy validation of the model. This could provide a basis for model enhancements that would improve future model performance at other sites. If needed, this information could also be used to re-estimate the time frame when remedial action objectives (RAOs) are expected to be met at the site.

WHAT IS MODELING?

Models and Their Uses

Starting with a Conceptual Site Model

The term "model" describes a broad range of tools that can be used to integrate and analyze available data. Models provide a framework for understanding site behavior and predicting the effects of actions taken at a site. A model can be as simple as a statistical regression, and as complicated as a process-based mathematical description of the physics, chemistry, and biology of a complex sediment site. Common to all models, though, is the need for a conceptual understanding of site behavior, i.e., a conceptual site model (CSM), which is a representation of the environmental system and processes determining transport of contaminants from sources to receptors.

At most Superfund contaminated sediment sites, the environmental system includes the food chain as a risk pathway for ecological receptors, humans, or both. Aquatic organisms can be exposed to contaminants in pore water, overlying surface water, sediments, and through their diet. Exposure to contaminants in sediments occurs primarily in the top layer (an "active layer" of sediment which can vary widely but is often on the order of 10 cm in thickness). Contaminants in deeper sediments can also serve as a source of contamination through their upward transport in pore water or erosion and reworking of the sediments by storms or other disruptive events that reintroduce them into the active zone. Contaminated sediment can be directly toxic to biota and can also serve as an entry point for food chain exposures to predators, anglers, and hunters.

To effectively manage and reduce risks due to sediment contamination, it is important to understand the processes that brought about those risks. This means understanding past and ongoing releases, the transport of chemicals in the environment, any changes in the form of those chemicals over time, and the pathways of exposure and risk to human and ecological receptors. This set of relationships linking releases to risk is included in the CSM. A CSM is formulated for every Superfund site, and site investigation supports the development, testing, and refinement of the CSM. In turn, the CSM can be used to identify gaps in the understanding of a site.

A CSM identifies the processes that lead to contamination and elevated risk and therefore need to be considered in remedial planning. These processes can be quantitatively understood and incorporated into a mathematical model, i.e., a set of quantitative relationships relating model inputs (e.g., initial conditions, boundary conditions, contaminant inputs, hydrometeorology, or watershed solids loads) to exposures and risks. While a mathematical model can improve the description of contaminant pathways and underlying processes, its primary purpose is to predict specific reductions in exposure and risk from potential remedial actions. It is often recommended that the CSM be developed into a mathematical model where sites are large and complex; where it is important to compare the effectiveness of remedial alternatives over long periods of time; and when a model offers an opportunity to support decision making.

Quantifying a CSM: Mathematical Models

Mathematical models include analytical models, regression models, and process-based numerical models. Analytical models include universal equations that provide a good fit to data without need for calibration using site data. Analytical models have limited applicability to contaminated sediment sites because of the complexity of processes and heterogeneity of conditions. Regression models provide a best statistical fit between independent and dependent variables. They can be useful in establishing relationships between variables from past data, such as the relationship between flow and suspended contaminants, or between sediment and fish tissue concentrations, but are limited in their power to forecast effects of remedial actions that change the character of the site, due to their reliance on past data. For these reasons, process-based numerical models can be the most useful mathematical models for contaminated sediments.

When there is a need to describe or forecast site behavior that cannot be captured with an analytical or regression model, a process-based numerical model is often applied. This is often the case in contaminated sediment systems. Sediment contaminants, especially organics with low water solubilities, tend to be strongly associated with solid particles, especially fine particles and particles that have a high organic carbon content. Those particles are often the products of watershed erosion, ongoing erosion of a river bed or banks, or naturally occurring organic materials. As flow rates vary through the year, those particles can be eroded from the sediment bed and moved downstream, and they can also be buried by other sediment. The amount of contaminant that is adsorbed to solids, dissolved, transported to the atmosphere, or transformed into other chemicals can be affected by a variety of physical processes, including hydrodynamics, the nature of the solids, temperature, pH, availability of oxygen, and biological activity. A numerical model can be used to describe those processes. Numerical models that describe physical processes can be combined with historical data on contaminant concentrations to simulate past, present, and future exposure concentrations at specific site locations. A wide range of numerical models exist that are capable of simulating physical properties and processes such as water surface elevations, velocities and shear stresses, solids concentrations and fluxes, contaminant concentrations and fluxes, and many other variables that may vary across large areas or long periods of time (Figure 1).

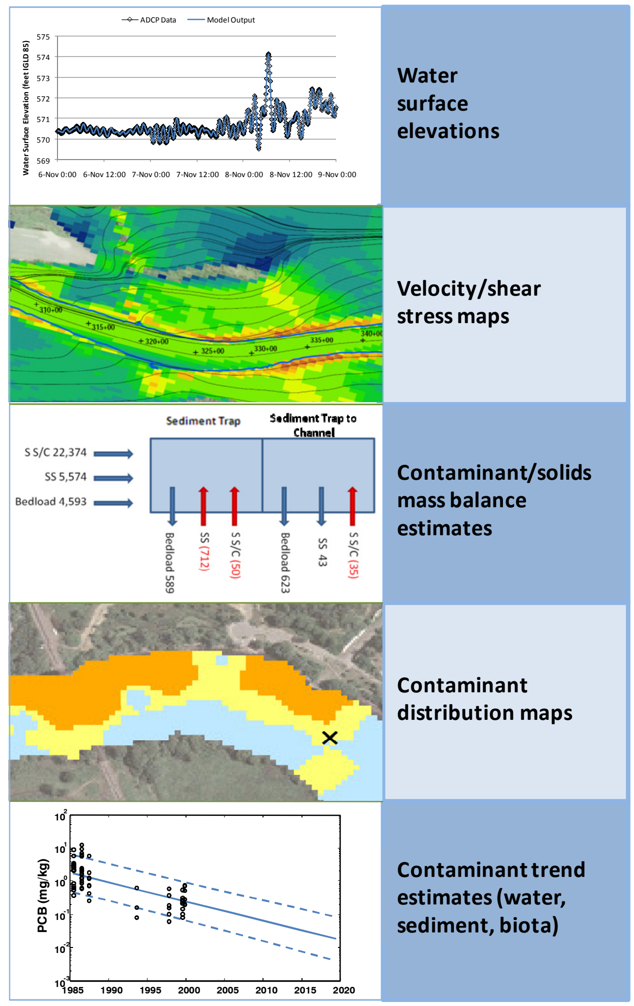

Figure 1: Example Output from Numerical Models Used to Simulate Various Physical, Chemical, and Biological Processes

Adding Complexity as You Go: Tiers of Model Development

As described above, the term "model" describes a broad range of tools with varying levels of complexity. Models can be classified into levels of increasing complexity, or "tiers", which provide increasingly detailed representations of the physical, chemical, and biological processes at work in a sediment system (Figure 2). The first tier includes simple empirical and statistical models useful for detecting statistically significant trends in contaminant exposure and exploring and testing for correlations among environmental variables (e.g., river discharge, temperature, water column contaminant concentrations, etc.). However, simple statistical models are inherently limited in their ability to predict future conditions. Such models typically are "fits" to available historical and contemporary data, and as such are unconstrained by the physics of the system being simulated.

The second tier builds on the first by using observations about trends and correlations, combined with an understanding of basic processes, to further develop the conceptual model of the system. For example, it may be possible to identify differences in the way contaminants in carp and smallmouth bass trend over time, and link those differences to known differences in feeding habits, thus linking differences to the degree to which each species is affected by contaminant trends in the sediment bed. Such observations superimpose knowledge of the physical behavior of contaminated sediment systems on empirical observations of the site captured in a Tier 1 model.

Tier 3 modeling involves organizing the knowledge of the masses of water, solids, and contaminants in different system compartments into a quantitative framework that measures fluxes into and out of these compartments and associated rates of accumulation in each compartment. By quantitatively tracking mass moving through the system, mass-balance modeling helps answer questions that are critical to evaluation of long-term trends, such as: What is the rate of accumulation of solids in the sediment bed? or, What is the rate of suspended solids and contaminant export downstream?

The complexity of the site, the scope of decisions to be made, or the specific management questions asked may require a more detailed modeling evaluation, often to provide an improved understanding of some critical piece of the system. A Tier 4 model is an extension of the Tier 3 mass-balance models that adds more detail or process modeling in important areas. This might include detailed, fine-scale and multidimensional hydrodynamics; a more mechanistic description of sediment transport and sediment bed handling; or a more mechanistic description of contaminant fate and transport processes. It might include the addition of other supporting modeling evaluations such as simulation of wind-wave dynamics, wind-induced currents, or extreme event modeling.

The decision to move from simpler to more complex models requires careful consideration of the need for and value of the added complexity. Increased model complexity can reduce decision-making uncertainty when used appropriately and when well supported by site data. If used poorly, added complexity can be misleading and can even increase uncertainty. A critical task for any modeling team, supported by experienced modeling consultants and other individuals not vested in the model development, is to carefully select a level of model complexity that provides real benefit and is appropriate to the resources available and the decisions being made.

Using Models

People who use and develop models often think of them primarily as prognostic tools – a way to predict the future conditions at a site. But when developed along with a project, starting simple and adding complexity as needed, models can support many other aspects of a sediment site investigation. Models from each of the different tiers of modeling described in Figure 2 can:

- Support directed data gathering during a remedial investigation
- Perform hypothesis testing and refine the CSM

- Act as prognostic tools for predicting future behavior of the system
- Support evaluation and selection of proposed remedies
- Support remedy design
- Help understand post-remedy monitoring data

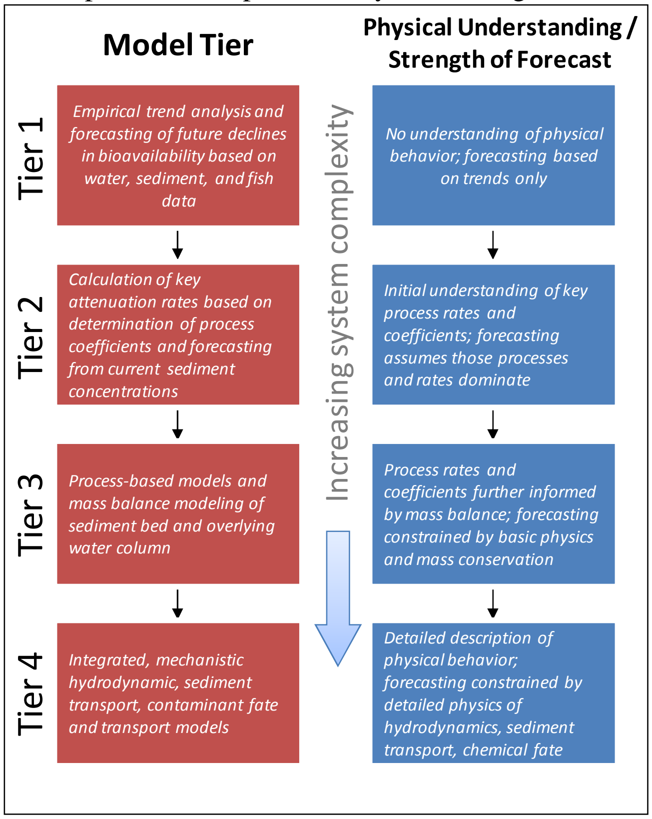

Figure 2: Tiers of Modeling Complexity

These activities can span the entire timeline of site investigation and remedy implementation. Models, especially simple models, can be used at the outset of a project to support planning for data collection, in the middle of a project to allow testing of important elements of the system behavior, and at the end of a remedial investigation to help choose between different remedial alternatives. And when a model is developed early, built with stakeholder input and peer review, and employed throughout the project, stakeholders can develop confidence in the value and utility of the model. This consensus will support its use when the project comes to the critical point of remedy selection and design.

Squaring the Model with the Data

Model performance is evaluated and improved by a process of *verification*, *calibration*, and *validation* (USEPA 2005). Every model should be carefully checked to ensure that it is based on accepted scientific principles and that there are no errors generated by faulty computer code. This process is called *verification*.

Models are based on data and scientific understanding of physical and chemical processes. Most of the equations in a model include numerical coefficients. To the extent that site data are available, some of the coefficients are based on the fit of the equations to data, and others are taken to be universal constants (the acceleration due to gravity being an example of the latter). Where site-specific data are limited, coefficients may be values from scientific literature. *Calibration* of a model is the process of adjusting its coefficients to attain optimal agreement between model-calculated values and actual site data. Most commonly, model calibration consists of fine-tuning the model to provide the best fit to site data.

The objective of calibration is to make the model as accurate as possible in its predictions. This accuracy is further tested through a process called *validation*. Normally in validation, a time period is simulated that is different from the period that was used to calibrate the model, and the model is run without changing any of the coefficients that were adjusted during calibration. This may require using only a portion of the data for calibration, thereby holding data from the remainder of the time period in reserve for validation. Calculated and actual values are compared, and if an acceptable level of agreement is achieved, the model is considered validated. If not, then further analysis of the model is performed, leading to refinements that should improve the accuracy of the model.

Persistent sediment contaminants can pose very long-term risks. The strong association of hydrophobic contaminants with flow-driven particles requires that models must be accurate with respect to flows and solids movements, in addition to the behavior of the contaminants themselves. For these reasons, calibration and validation datasets should ideally cover long enough time periods to capture the range of variability of flow, extreme events causing erosion, and measureable sedimentation. This is needed to ensure the model's accuracy with respect to the build-up and erosion of buried contaminant deposits. Fitting the model to shorter time periods and more limited data targets can give a false impression of predictive accuracy. For sites with limited historical data where it has been decided that a mathematical model is needed, it is important to begin collecting needed data as soon as possible.

The concepts of model calibration and validation are illustrated in Figure 3, where a hypothetical model's development and application is depicted in terms of modeled surface-weighted average concentrations (SWAC), an example of a spatial interpolation method. The model is initiated with a dataset describing initial conditions, calibrated to a dataset spanning a long (e.g. 20 year) period, and validated against data collected at the end of the calibration period. The model can then be used in two predictive capacities, as a hindcasting tool to simulate how contaminant levels and exposures likely changed historically before the calibration period, and as a forecasting tool to predict future changes to the system. In this example the model is used to simulate three remedy alternatives: a Monitored Natural Recovery (MNR) alternative that monitors the system as naturally occurring processes reduce sediment concentrations; a dredging alternative that causes a short-term increase in sediment concentrations, followed by a general decrease and continuing recovery due to natural processes; and a capping alternative that reduces surface sediment concentrations by adding an engineered layer of clean material.

Uncertainty in the model's prediction of SWAC is represented by the two sets of dotted lines that bound the upper and lower range of predicted concentrations for the two simulated remedies. The uncertainty bounds are tightest in the calibration and validation periods, where data are richest and constraints on the model are the greatest. The uncertainty increases as the hindcast and forecast extrapolate further from the calibration period. The topic of uncertainty is discussed in greater detail in a following section.

Models integrate data and scientific knowledge to better understand the connection between contaminant releases and risk at a specific site. Models do not create data, but should be consistent with available data, for which they provide a means of synthesis and understanding. Ideally, model formulation should proceed in tandem with the site investigation. The CSM can identify media, processes, and locations of greatest interest and focus the data collection effort. This ensures that the resources devoted to site investigation provide information that is useful for risk management and remedial planning. In turn, data from the site investigation can be used to test the conceptual model's hypotheses and to improve the predictive power of a mathematical model.

Models are Approximations with Specific Objectives

It is important to recognize that all models simplify complex processes, and that the objective of modeling is to adequately represent the processes of greatest importance, rather than fully describe every aspect of sediment contamination. (USEPA, 2008a, Glaser and Bridges, 2007). Just as a good map shows key features and suppresses unwanted detail, to highlight the information needed for the map's intended purpose (compare, for example, a road map and a weather map), a model includes

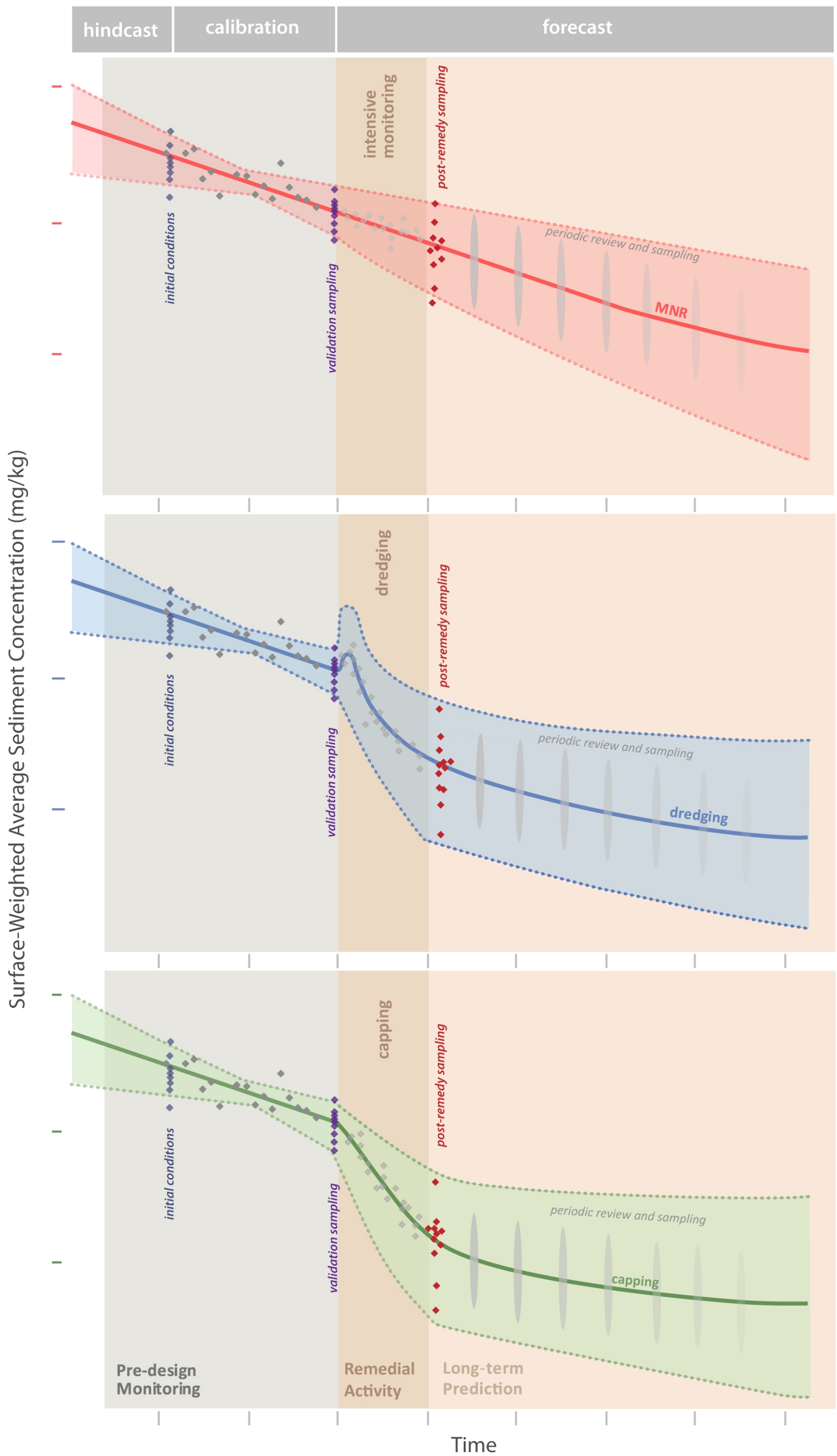

Figure 3: Model Application to a Remedy Evaluation: Calibration, Hindcasting and Forecasting

(Note: Dotted lines represent 95% confidence intervals for predicted average concentrations) representations of key processes needed for specific objectives. This makes models practical tools for problem solving, and at the same time ensures that they will never fit data perfectly. In addition, there are real gaps in scientific understanding of natural systems, and practical computational limitations on simulating events at the very fine space and time scales at which real processes take place, especially when long-term forecasts are required. A model should be thought of as an approximation of reality, representing the processes that are most important for making realistic predictions of exposure and risk over the time frame of concern. "Models will always be constrained by computational limitations, assumptions, and knowledge gaps. They can best be viewed as tools to help inform decisions rather than as machines to generate truth or make decisions." (NRC, 2007a) By using the best scientific understanding to select and represent key processes, it is possible to forecast the future under various remedial scenarios, and to evaluate relative risks.

WHAT'S IN A MODEL?

Elements of Models

Contaminated sediment sites are dynamic systems in which exposures can change over time due to human activities and natural forces. Contaminants are usually present in multiple forms such as dissolved, particulate, and vapor-phase, all of which have the potential for exposure to receptors. The contaminants that persist in sediments are those that tend to adsorb to solids, with smaller fractions in dissolved and vapor phases. A model of potential exposures due to sediment contamination tracks the contaminant as it is distributed among these different physical forms, and as it is transported into, out of, and around the site.

Contaminant transformation and transport is typically driven by natural processes. For example, the change in the water column concentration of an adsorbed contaminant (*i.e.* on suspended solids) on any given day depends on inputs that include any ongoing contaminant loads, the flow rate, and the temperature. A model of adsorbed concentration expresses how contaminant concentration rises and falls from day to day as a function of these other variables. In this example, adsorbed contaminant concentration is an indicator of the state of the dynamic system, a *state variable*. The concentration of dissolved contaminant in surface water is another state variable. Changes in sediment loads, contaminant loads, and weather force changes in state variables and are therefore called *forcings*. When we express forcings as functions of time (such as a series of daily flows or temperatures) they are called *forcing functions*. Because contaminant concentration is dependent on the other variables, it is called a *dependent variable* and the variables that affect it are *independent variables.* A summary of some of the major components of a typical sediment, contaminant, and fish bioaccumulation model is presented in Figure 4.

Complexity and Scale of Models

At the outset when developing a model, decisions must be made about the degree of complexity that is justified. Simple models are more easily understood by scientists, decision makers, and the public and they may provide a reasonable degree of accuracy for minimal investment.

Complexity can provide added utility, but at the cost of time and resources, and its utility depends on the questions asked and the expected benefit of answering them more accurately. More complex models require more effort to construct and more data to fit. However, if a complex model is not appropriately constructed and tested, consistent with management questions and supporting data, it cannot provide better answers; it will only be more difficult to understand, take longer to develop, and cost more. As noted previously, managing the complexity of a model and keeping the focus on model utility is a critical task to be addressed by a modeling team and their consultants. The EPA Superfund Sediment Resource Center (SSRC) provides valuable guidance and support to project teams. (http://www.epa.gov/superfund/health/conmedia/sediment/ssrc.htm)

The questions to be addressed using the model may be relatively qualitative (could sediment be transported from point A to point B?) or more quantitative (how much sediment and associated contaminant is transported every year from point A to point B, and what is the trend, if any, in those amounts?). A remedial project manager (RPM) should decide whether a qualitative or quantitative answer is needed, what project resources are available to support the decision, and consequently what level of complexity in analysis or modeling is appropriate. It is always good practice to ask "if we add a level of complexity, what (if anything) can we simulate more accurately, and how will that improve management decision-making?"

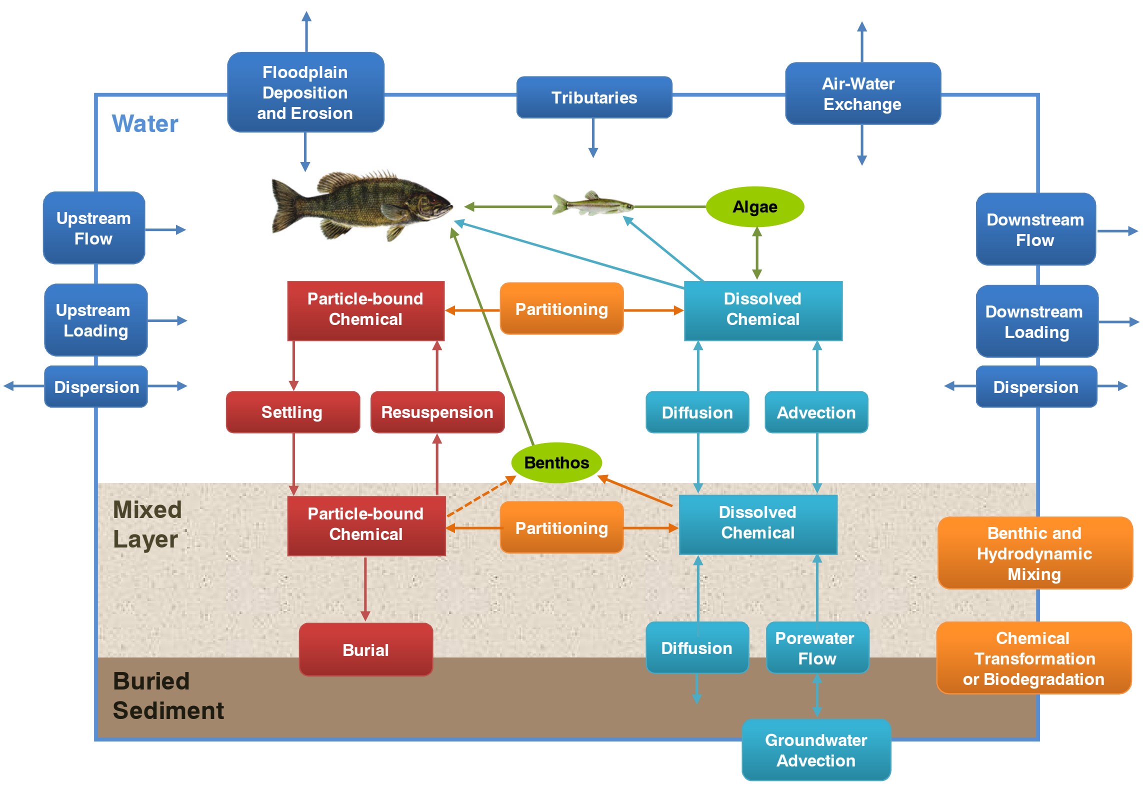

Figure 4: Simplified Summary of Processes and Variables in a Contaminant Transport and Fish Bioaccumulation Model

Dimensions of Model Complexity

Dimensions of complexity include *statistical versus mechanistic*; *coarse vs. fine*; *steady-state vs. dynamic*; and *deterministic vs. stochastic*. Statistical (sometimes termed "empirical") models, such as the regression models discussed above, rely on observed correlations between variables rather than mathematical representations of known physical, chemical, or biological processes. Statistical (Tier 1) models are simple to construct and apply, but are suspect if conditions change relative to the period of data collection. Mechanistic process-based (Tier 2-4) models are more burdensome to construct, but can be more accurately descriptive, and if processes are correctly specified they can help to extend forecasting outside the range of current site data. Most models employ a mix of statistical and mechanistic equations, with the split depending in part on which processes are well enough understood to formulate mechanistically.

Choices also need to be made about coarse vs. fine resolution, in both space and time. Spatial resolution amounts to the sizing of model grid cells. In a sediment transport model, cells usually extend down vertically as well as covering the site horizontally. Time resolution is the degree to which the simulation period is divided into incremental units of time, or time steps. The forecast for an individual cell and for a particular time step represents an average over the whole cell and time interval, even though there is real variation in each dimension. Cells and time steps should be fine enough that forecasts for particularly important points in space and time are not lumped with neighboring areas and time periods. Significantly more input data are needed to support higher resolution, and resolution should be increased only as needed, in a way that improves the value of the model as a hypothesis testing and remedy evaluation tool.

Steady state modeling assumes constant forcings and produces constant values of state variables, whereas dynamic modeling allows forcings to vary over time, with resulting dynamic behavior in state variables. For some purposes, such as identifying the strength of relationships between variables, steady-state modeling can be simple and instructive. For example, steady state simulations at two different flow rates, all else held equal, can produce a clear illustration of the effects of different flows on sediment transport. However, variability can be important in itself. An example is the tendency of recently deposited sediment to erode during rising flows. At the tail end of an event, the opposite occurs, with sediments depositing, and a steady state simulation could not capture both phenomena.

Much modeling is deterministic, which means that a single value is determined for each dependent variable in each forecast period, intended as a best estimate. In contrast, stochastic modeling produces ranges of forecast values. When inputs are uncertain but their uncertainty bounds are known, this information can be used to generate a range of forecast values. Depending on the project, there may or may not be value in understanding this range, and the modeling team needs to assess the value of adding a stochastic model. When avoiding worst cases is of great concern in planning a remedy, stochastic modeling can be very useful in estimating the likelihood of those worst cases. But as with any modeling exercise, the value of stochastic modeling should be weighed against the additional cost of developing stochastic simulations.

The most useful models are not necessarily the most complex, they are models that are best designed to answer site management questions. The best compromise between simplicity and complexity always depends on the specific questions asked of the model, the resources available to build and run it, and the degree of certainty needed. These factors and their implications for modeling vary considerably from one site to the next, and should be evaluated on a site-specific basis.

Linked Models for Sediment Sites

Models used for sediment management often comprise linked models of water, sediment, contaminants, and biota. There are many sediment and chemical fate and transport models available today, describing a broad range of processes, with widely varying degrees of complexity, and many different authors and levels of support. Similarly, food web models are numerous and vary greatly in complexity and in ease of use. A brief summary of major categories of models is provided in this section, and examples are listed in Appendix A.

Hydrodynamic models of flow use flow records taken at fixed gaging stations and/or downstream receiving water levels, both of which are forcing functions for the model. Hydrodynamic models take into account the bathymetry (depth and width) of the water body, subdivide the waterbody into a grid of model cells, and route the input flows from upstream to downstream from one cell to the next. The purpose is to predict local velocities, which may increase or decrease depending on changes in bottom slope and cross-sectional area. Hydrodynamic models depend primarily on the physics of water flow, considering the effects of flow inputs such as watershed flows, tributaries, groundwater-surface water interactions, and lake or ocean boundaries, and taking into account local friction due to bed roughness, vegetation, or engineered surfaces. Hydrodynamic models of rivers can usually be closely calibrated to data on water levels or stream velocities.

Inputs of solids are carried into the system by flows, and can deposit as bed sediment at lower flows and resuspend at higher flows. The relationship of solids movement to flow is described by a *sediment transport model.* Solids inputs from upstream and from smaller tributaries are a key forcing function for the sediment transport model. The sediment transport model describes how those solids are transported downstream over time in the form of suspended load or bed load. Bed load is a movement of solids skipping and rolling along the sediment bed, whereas suspended sediments are distributed by turbulence from bottom to top of the water column.

Like the hydrodynamic model, the sediment transport model divides the sediment bed into cells so that it can make local predictions about sediment accumulation or erosion. It may also include vertical layering to predict changes in sediment bed elevation over time. A sediment transport model uses the local velocities provided by the hydrodynamic model to predict local erosion or sedimentation of solids. In general, sedimentation is simulated in models at the lowest velocities, when velocities are too low to keep sediment in suspension. Erosion is simulated in models when the bottom shear stress created by flow reaches a critical level, and greater erosion rates occur at higher velocities. Sediment transport models can be calibrated to concentrations of suspended sediment and to measured erosion and bed sedimentation rates.

The movement of sandy sediments is better understood scientifically and easier to predict with equations than the movement of finer particles like silts and clays. This is because the cohesiveness of those smaller particles is a complicating factor and differs from site to site. The movement of sand particles in response to flows can often be described by standard textbook equations that are applicable at any site. For silts and clays, however, the tendency to erode depends on complex characteristics of the local sediment, and has not been fully explained in terms of simple, measurable properties (like bulk density and grain size). Consequently, the equations that models use to describe erosion are often based on direct measurements of local erosion. Ideally, these measurements are made with flumes placed on the sediment bed or operated in a laboratory, applying a flow to erode sediment samples collected at the site. If flume measurements are not available, standard erodibility equations can be calibrated to data on suspended sediment concentrations measured at varying stream velocities, but are subject to greater uncertainty in forecasting. Models of erosion of cohesive sediment also take into account the age of sediments, such that fresh sediments are predicted to erode more easily than sediments that have had days or weeks to consolidate.

The hydrodynamic and sediment transport model components set the stage for modeling of *contaminant transport*. Contaminants can be dissolved, associated with solids, or can occur in the form of a gas. They can also be associated with colloids, which are suspended solids that are so fine that they do not settle at the lowest velocities. Contaminant transport models include a partitioning component that determines how much of the contaminant appears in each form in the sediment bed, including the pore water that surrounds sediment grains, in groundwater that may pass through the sediment bed, and in the overlying water column. The bed and water body are divided into a grid of model cells, and a set of partitioning calculations is performed to distribute the contaminant in each cell into its various forms. Partitioning calculations are usually based on published partition coefficients that describe a chemical's tendency to adsorb to solids, dissolve, or occur as a gas. These coefficients are chemical-specific, but the hydrophobic organic chemicals that are the targets of many sediment clean-ups are primarily associated with solids, especially with fine-grained material having a high organic carbon and/or black carbon (*e.g.,* soot and char) content. The relationships used by models to describe those strong associations between organics and solids depend on the organic carbon partition coefficient (K_{oc}) and on the organic carbon content of solids. Predicted concentrations in each form and location can be compared to actual contaminant samples from those media, and the model calibrated to more closely predict those concentrations.

Site-specific measurements of partition coefficients should be used if they are available. If not, which is often the case, a comprehensive handbook of chemical-specific partition coefficients. such as K_{ow}, K_{oc}, and Henry's Law Constant (H) is Mackay, *et al*., (1992), now available in a continually updated CD-ROM from CRC press. EPA also supports a set of software products, called EPI Suite, that can be used for estimating many of the chemical-specific parameters used in models if site-specific measurements are not available (http://www.epa.gov/opptintr/exposure/pubs/episuite.htm).

Often mixtures of chemicals, such as total PCBs or PCB homologs, are modeled. In this case, it is most desirable to obtain site-specific partitioning measurements, followed by minor adjustment during model calibration (Bierman *et al*., 1992; Butcher *et al*., 1997). If that approach is not possible, a partition coefficient value for these mixtures may be estimated by weighted-averaging of the literature values for the individual chemicals found in the mixture.

Models of metals contamination also use equations to represent partitioning to solids versus the dissolved form. Partitioning of metals to solids can depend very strongly on oxidation-reduction conditions in the sediment. In oxygen-deprived sediments, sulfur appears in the form of sulfide and bonds with metals to form insoluble sulfide compounds. Where oxygen is more abundant, sulfide is transformed to sulfate and metal ions are released and can occur in dissolved form.

For both organics and metals, partitioning is a key to bioavailability. Sediment-dwelling organisms, for example, may be much more vulnerable to pore water contamination than to contamination that is tightly bound to sediment particles. Partitioning also affects transport from the source area to downstream and downwind locations. This includes dissolved contaminant traveling downstream at a rate that is predicted by modeled water flow, and contaminant that is adsorbed to solids, moving with those solids as they settle, resuspend, and travel in suspended form.

In some cases, particularly low- flow conditions, groundwater may be a pathway for transport of contaminants through the sediment bed. While groundwater models may be of importance in characterizing groundwater-surface water interactions in sediment models, their use is not detailed in this document. An additional process that is usually modeled as a loss to the aquatic system is contaminant in vapor form escaping to the atmosphere and transported away from the site. At some sites, air is a significant exposure pathway, and in such cases concentrations in ambient air should also be simulated.

While direct exposure to contaminants may pose risk, the most important risks to human and ecological health can arise through bioaccumulation. *Food web models* translate the dissolved and adsorbed concentrations provided by the contaminant transport model into body burdens for target ecological receptors, including fish and wildlife species, and the species that comprise the food chain that sustains their populations. (As an example, Figure 5 shows results from a food web model developed for PCBs in the Lake Ontario ecosystem.) Food web models represent populations of birds, fish, and their prey by age cohort and area. The accumulation of contaminants in organisms is essentially the difference between contaminants accumulated via food and water and contaminants lost via respiration and excretion.

In food web models, the contaminant is bioaccumulated as a byproduct of obtaining energy through food, and the fraction absorbed by the body is governed by a partitioning equation, similar to the partitioning between water and solid particles. Partitioning to tissue depends on the fat (lipid) content of the organism, just as solids partitioning depends on organic carbon content (see more detail on page 18). Some food web models also simulate foraging as movement between available habitats in response to their characteristics and availability of food. “Static” applications of foodweb models depict organism contaminant concentrations at a point in time under specified conditions. “Dynamic” applications simulate changing concentrations in the organisms over time. As individuals are simulated to age and grow, they build up contaminant in their tissue. In this way, food web models represent the accumulation of contaminant over the life cycle of the organism, simulating real-life relationships between age, size, and location of biota and their contaminant body burdens.

With data on current conditions and the combination of hydrodynamic, sediment transport, contaminant transport, and food web models, future tissue concentrations for target species can be forecasted. A forecast simulation begins with a set of initial conditions, including estimates of current contaminant concentrations in sediment, water, and biota.

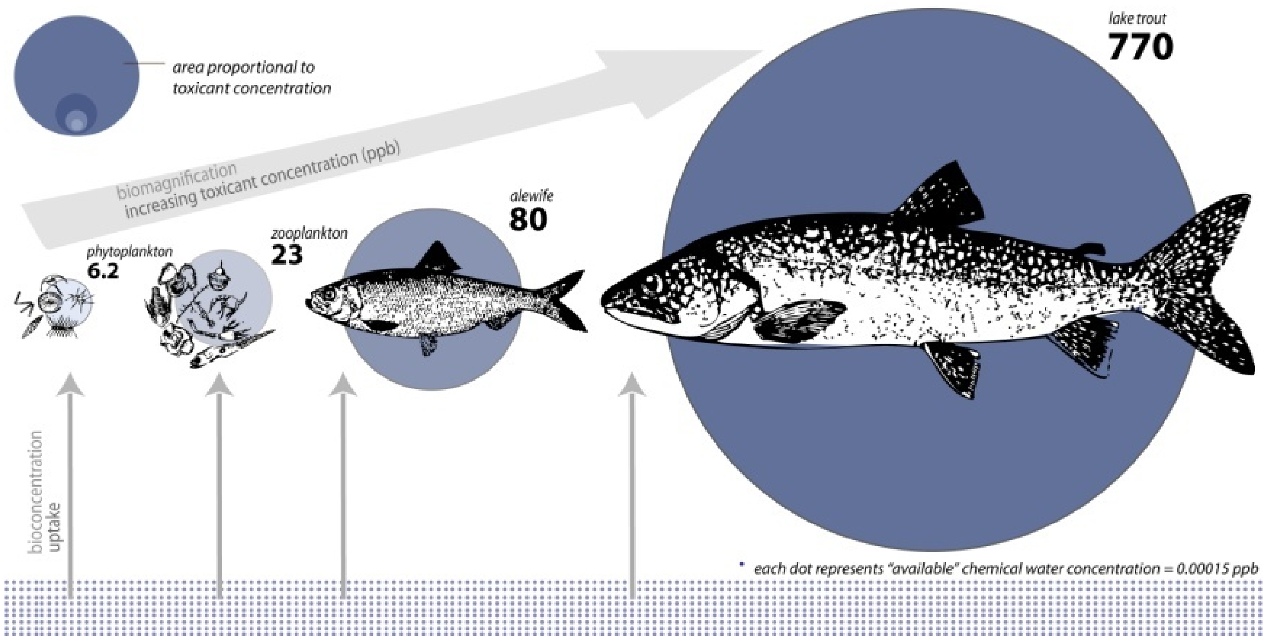

Figure 5: Bioaccumulation of PCB in Lake Ontario

With linked models, initial conditions are often defined at different spatial scales. A river reach may have many model cells, with the initial conditions in each cell based on sediment samples obtained within that cell, whereas a food web model may represent the same reach as a single model cell, with initial conditions based on fish sampled throughout that reach.

Additional inputs required as forcing functions include long-term daily series of any ongoing contaminant loads, based on best judgment about future source control, and of future solids loads, flows, and temperatures. Assumed solids loads will depend on assumptions about future watershed development and management, and flows and temperatures are derived from the historical record and can be adjusted to reflect any expected changes in conditions.

The model proceeds from one time step to the next, routing stream flows through the system, moving sediment, partitioning and transporting the contaminant downstream, and simulating biological uptake of contaminant.

The result of the forecast is a prediction of the spatial pattern of contaminant exposure and bioaccumulation as it develops over time, reflecting the effects of legacy contamination and changing conditions. This may include increasing exposure due to erosion and/or decreasing exposure due to burial of the contaminant.

When this forecast of exposure is combined with other exposure and effects data, such as frequency of fish consumption and health risk factors associated with the contaminant, the result is a forecast of risk as it can be expected to change over time, *i.e.*, under the no-action and MNR alternatives.

To evaluate the potential benefits of remediation, a similar forecast can be generated with updated bed conditions, reflecting concentrations that are expected to be present after a remedial action. The difference in the two forecast outcomes, with and without changes in assumed bed conditions due to remedial action, represents the expected net benefit of remediation. The time pattern of those predicted benefits may reflect tradeoffs between present and future: for example, a dredging remedy is likely to cause some sediment resuspension and contaminant release and transport initially, but may lower future exposures and risks, in addition to removal of some of the contaminant mass. The use of models to predict remedial outcomes is described in greater detail in a following section.

Process Representation in Models

Models provide a framework by which many different physical processes can be identified, quantified, and compared in terms of their relevance to a particular risk management endpoint. For example, processes like particle settling and deposition, event-based resuspension, and bioturbation may all be important in controlling how contaminant levels in surficial sediments change with time. Or, if a goal at a particular site is to limit present and future exposure of a particular fish species to sediment bed contaminants, models can assess the processes that control that exposure, and identify which processes or parameters actually matter most. The example below highlights how model development and revision can inform exposure processes, risk assessment, and remedy selection.

Example:

Problem: In a slow-moving river in a mostly agricultural watershed, sediments downstream of a historical chemical waste recycling operation show elevated levels of PCB at 3-4 feet of depth, and lower contaminant levels at shallower depths. Measurements of the age of sediments at depth were made using geochronological dating methods. MNR is proposed as a remedy alternative to limit exposure of benthic feeders to surficial sediments.

Model Application: An Environmental Fluid Dynamics Code (EFDC) model is constructed using measurements of upstream suspended sediment concentrations across a range of river flow rates to provide an estimate of solids load to the upper river. A problem arises during model calibration: when the model is calibrated to present-day suspended sediment levels throughout the river, the predicted rate of sediment deposition and burial isn't high enough to explain the depth of burial of the contaminants, given what's known about historical contaminant releases.

Conceptual Model Revision: Further exploration of the upstream solids load shows that historically, solids loads were much higher because there were fewer agricultural runoff controls in the 70's and 80's. A revised model that incorporates a long-term trend of decrease in upstream solids load is used to reproduce historical deposition and forecast the future rate of burial of bed contaminants.

Outcome: The model shows that the sediment recovery rates predicted by geochronological cores probably overestimate the present-day rate of recovery of the system, due to the expected continuing decrease in upstream sediment supply and its effect on sediment deposition in the vicinity of the PCB deposits. The MNR assessment is adjusted to reflect a slower rate of recovery than initially envisioned.

WHAT'S NEEDED FOR A MODEL?

When a site is listed on the National Priorities List (NPL), there is typically some information and data on the extent of contamination. Sources may have been identified, and specific ongoing migration pathways may be suspected. To refine this thinking into a solid CSM, and to build a process-based numerical model if appropriate, additional data are needed. Ideally, those data can be used to quantify any continuing sources of contamination; tabulate the range of water flows in the contaminated area; show how solids move between the sediment bed and a suspended state at various flows; determine how much of the contaminant is dissolved and how much is attached to solids; and show how much contaminant is taken up by target fish and wildlife species through their life cycle. Through data collection, each link in the CSM is tested and verified or refined.

Data collection is costly and its purpose is not to be exhaustively descriptive of the site. It should be carefully targeted to the key sources, pathways, and exposures in the CSM, especially those that are key site-specific determinants of human health and ecological risks. If this is done effectively, then the data set will support model construction, and model development will also assist with identifying data needs. On the other hand, if there is not enough thought given to these conceptual links in the data collection phase, then the task of predicting the effects of remedial management actions will be much more difficult, whether or not this is done with a numerical model.

Sediment Data

Modeling begins by quantifying current contaminant inventories in sediment, and other sediment characteristics that can affect concentrations and sediment stability. These are the model's *initial conditions.* The following is a representative set of data to collect on sediment, described in greater detail below:

- Contaminant concentrations
- Organic carbon content
- Acid volatile sulfide (AVS, when metals are present at concentrations that may pose risks)
- Dry bulk density (g/cm^3 dry weight)
- Grain size distribution

Sediment sites can be vast, and sampling is costly, so the sampling plan should be carefully designed to provide good coverage, both horizontally and vertically, of contaminant deposits, while collecting only the data needed to support a risk management decision at the site. Sediment core samples are preferred to surface grabs because it is important to include subsurface sediment characteristics, including contaminant concentrations, in models. In the vertical, cores should be segmented in such a way that vertical layering and lower bounds of deposits can be identified. This depth could be based on an estimate of the historical rate of burial (such as from navigational dredging records) and knowledge of the dates of release. Judicious analysis of a subset of core segments and archiving of others can minimize the analysis of uncontaminated samples at depth.

In the horizontal, samples should be distributed so as to try to capture concentration peaks and trends. It is a fact of life for large sites that sediment core data will be used to represent large areas between cores, with uncertainty about sediment concentrations at unsampled intermediate locations.

Sediment organic carbon content is important to analyze because of the chemical affinity between it and nonpolar organic chemicals. This strong affinity makes organic contaminants less bioavailable, thus decreasing contaminant bioaccumulation in organisms. The situation is similar for metals in sediments with high sulfide content. In this case, metals tend to be present in insoluble form, and are much more difficult for organisms to assimilate in tissue than in dissolved form. These differences in bioavailabilty are important from a risk perspective.

Bulk densities and grain sizes are important in predicting erodibility. Sediment with lower bulk density is generally more easily eroded. For grain size, coarse particles (sands and gravels) are less erodible than finer particles. Fine-grained sediment, which includes a high proportion of silt and clay, forms a cohesive bed and erodibility is highly site-specific, as discussed on pages 12-13.

Hydrodynamic Data

Data required for *hydrodynamic models* include inflows, physical boundaries of the water body, and any water levels that can be considered fixed for purposes of the model. Typical river flows, for example, depend on flows from upstream and from tributaries, the geometry of the channel, and the water surface elevation of a downstream water body. The most basic predictions of these models are velocities and water levels, so those data are needed as targets for calibration. Thus, the dataset to build a hydrodynamic model will typically include:

- Bathymetry and shoreline geometry
- Upstream flows, preferably from a reliable gage with a lengthy historical record
- Watershed drainage areas for important ungaged tributaries
- Water levels at any downstream boundaries (*e.g.* river, lake, or tidal boundary), preferably from a reliable gage with lengthy historical record
- Stream velocities
- Water surface elevations

Bathymetric information and shoreline geometry can be collected at a very fine scale, but the degree of hydrodynamic model refinement should still be governed by the anticipated use of the model. For example, if it is important to estimate stream velocities and associated erosive forces for local site features of a specific size, to support remedial planning, then the grid in that area should be refined. However, an overly fine hydrodynamic grid could cause model run-times to be excessive without adding significant accuracy to forecasts of sediment and contaminant transport.

Data on Solids, Erosion, and Deposition

Data required for *sediment transport models* include information on the solids in the sediment bed, as initial conditions, and solids in suspension and moving along the bed as bed load, as calibration and validation targets. It is important to understand the movement of sediment under normal day-to-day conditions and during extreme events. Outputs of the hydrodynamic model, including water depth, velocity, and shear stress, are also inputs to the sediment transport model, Suspended solids and rates of bed erosion and sedimentation are outputs of the sediment transport model that can be compared to data for model calibration and validation. A basic dataset to build a sediment transport model will typically include:

- Water column samples of suspended solids, sampled over a range of flows
- Bed load flux rates and physical properties, if bed load is present
- Flume studies of erodibility at high velocities and shear stresses
- Long-term measures of erosion/deposition

Water column suspended solids data should be collected at enough stations on the water body to capture any longitudinal changes in suspended solids due to erosional or depositional areas. Bed load, if present, can be quite local, and bed load samplers should be deployed along transects with close spacing.

Flume studies can be used to provide a measure of the erodibility of sediments. They are generally unnecessary with noncohesive sediments (sands and gravels), whose properties are well-known, but are valuable with cohesive sediments (silts and clays) because their erodibilities vary considerably from site to site.

In contrast, long-term erosion/deposition data provide an integrated look at changes in the sediment bed over the full range of high and low flows that have occurred. These rates can be inferred from successive bathymetric studies, navigational dredging records, sediment traps, erosion pins or chains, and analysis of vertical distributions of certain radioisotopes (notably Cs-137 and Pb-210) in sediment cores. These measurements can be highly variable from year to year and location to location, so the use of several types of data from several locations is strongly encouraged.

Flume studies and measurements of long-term erosion and deposition should employ samples and data from enough locations to provide a representative picture of sediment erodibility for distinct areas of the site. This includes uncontaminated as well as contaminated areas, because sediments eroded from uncontaminated areas can contribute to burial of contaminants in downstream portions of the site.

For eutrophied waterbodies, algal solids can serve as another solid transport medium for solids. A model of algal solids growth is an important piece of the overall solids balance in these cases. These models are complex, and require data on nutrients and sunlight as inputs, and chlorophyll as a calibration target.

It is important to stress that the data required to support an extensive sediment transport modeling effort can be difficult and expensive to collect. Sediment transport is often strongly impacted by high flow events, which can be very difficult to monitor and often produce highly transient data that can be challenging to interpret. Sediment characteristics that affect transport are typically highly heterogeneous, and that heterogeneity can drive extensive data collection efforts if not limited by careful consideration of the real needs of the project and the modeling required to support it. For sediment transport modeling in particular, it is critically important that the project team carefully consider the level of model complexity required to answer project questions, and the corresponding degree of data richness and resolution required to support model development.

Contaminant Data

Hydrodynamic and sediment transport models predict the downstream movements of water and solids. A *contaminant transport model* builds on those predictions to simulate the transport and environmental fate of the contaminant. The initial conditions describe the initial mass, extent, and distribution of the contaminant. Its predicted fate and transport is then governed by partitioning to water and solids (*i.e.,* to particulate organic matter and inorganic sediment) as they move through the system. Snapshots of adsorbed and dissolved contaminant concentrations at several locations in the water body on sampling dates that span a representative range of flows serve as calibration targets. Additional data required for contaminant transport models include:

- Partitioning coefficients for chemicals of concern (typically from literature or handbooks), including K_{oc} and the Henry's constant governing volatilization

- Dissolved, colloidal, and adsorbed concentrations of contaminants in the water column, sampled over a range of flows and temperatures

Like suspended sediment samples, water column contaminant samples should be collected at enough stations to capture longitudinal changes due to erosion and deposition. In cases where pore water plays a significant role as an exposure or transport pathway, pore water sampling may be a useful additional source of information (USGS, 1998).

Biological Data

Food web models build on predictions of flows and contaminant concentrations, adding contaminant uptake by local biota. To do so the food web model needs to simulate local populations of representative food web species, including their dietary preferences and contaminant exposures. Tissue concentrations are the calibration targets for these models. Typical data for food web models include:

- Identification of endpoint species, diet, and predator/prey relationships
- Tissue contaminant concentrations, along with data on model inputs including age, size, and lipid, moisture, and solid contents of organisms
- Temperature and dissolved oxygen concentrations

Biota are exposed throughout their home and feeding ranges, so sampling should target species that are not exposed to contamination outside the site that is to be remediated, to give a clear indication of local exposure and uptake. Tissue concentrations can be highly variable, and numbers of organisms sampled should be planned carefully to ensure that their medians or averages are representative of the population, with acceptable standard errors. If data are collected in successive rounds, variances from initial data can be used in planning sample sizes for subsequent rounds (USEPA, 2008b).

It is worth reiterating that data collection is costly, and no dataset can form an exhaustive description of the entire system. Data collection resources should be focused on the sources, pathways, and/or exposures that are most important from the standpoint of risk reduction, and that are least well understood. Data collection is justified to the extent that it can help in understanding these relationships, especially as that understanding informs remedial decision-making.

Single Versus Multiple Rounds of Data

Important sediment and contaminant processes take place over a range of time scales. Stream flows vary daily, weather conditions vary seasonally, and long-term changes in the sediment bed take place over periods of years. Depending on the requirements of the investigation, data collection activities may focus on short-term fluctuations, seasonal changes, or long-term trends.

Short-term data are important for understanding variability in exposures, especially changes due to flows, including extreme flow events. A model based on short-term data is best suited to simulating the near-term range of potential exposures, given expected frequent variations in flow and temperature, assuming implementation of alternative remedies. Data collected over multiple years are essential to making realistic predictions of long-term trends in sediment and tissue concentrations. This understanding of trends is especially important in predicting the long-term effects of remediation, because all remedies depend to some extent on natural recovery processes, and these processes take time. Collecting multiple rounds of data on concentrations in surface sediments, water, and biota, from the commencement to the completion of the site investigation, provides the clearest picture of long-term trends, which can serve as long-term calibration targets for models and improve the accuracy of forecasts of the time needed to achieve long-term remedial targets (Figure 3).

Models and Data Collection

Everyone knows that models need data, but what's less well known is that data collectors need models. An initial site investigation that is guided by an accurate conceptual understanding of system behavior (a conceptual model) is likely to be far more efficient than a purely exploratory data gathering effort. And, a site investigation that builds on previous phases of investigation and model development can be highly targeted, making measurements only where needed, as guided by the model. Models provide a framework for organizing data, and for testing consistency with other sources of data and physical processes that govern site behavior. And in turn, collected data provides the basis for further model development and refinement. The example below illustrates how data gathering and model development can proceed hand-in-hand at a contaminated sediment site.

Example:

Background: A long-term dataset of fish contaminant levels collected at a contaminated sediment site shows a long-term trend of decreasing body burdens with time. In order to better understand the relationship between fish contaminant levels and sediment concentrations, a model is developed in the Gobas framework, drawing on the existing dataset of surficial sediment contaminant levels, fish body burdens, and a limited set of benthic invertebrate data. A parallel laboratory investigation is conducted to develop biota-sediment accumulation factors (BSAFs) for bottom-dwelling fish using site-specific sediment samples.

Model Application: Predicted fish body burdens, based on a Gobas model calibrated to fish and sediment data from the site, indicate less bioaccumulation than predicted by the laboratory-based BSAFs. The generally lower site fish body burdens suggest that the mode of exposure to sediments may be affected by spatial variability in contaminant levels and fish habitat preferences, making it worthwhile to account for differential exposures by habitat type in the food web modeling.

Additional Data Collection: A sidescan sonar survey of the sediment bed shows significant variation in the texture of the bottom substrate and the associated habitat quality. A series of electroshocking surveys exposes a strong fish preference for irregular bottom structure, particularly rocky substrate where contaminant exposure is lower than in broad areas of sediment where deposited fines have high levels of contaminants. Incorporation of these findings into a version of the Gobas model that accounts for such preferences results in a reduction of scatter in model calibrations, improved predictive capacity of the model, and reconciliation of model results with laboratory BSAF studies.

Outcome: The strong habitat preference expressed by the target species results in a reassessment of remedies, with a greater emphasis placed on habitat improvement paired with reductions in exposure concentrations.

HOW CERTAIN ARE MODEL PREDICTIONS?

Models make predictions with uncertainty for a number of distinct reasons. This section will catalog those sources of uncertainty, and discuss how to quantify their effects on forecasts, as well as what level of uncertainty is reasonable to expect.

Sources of Uncertainty

One category of uncertainty is *model uncertainty*: the equations of a model may not fit the true physical, chemical, or biological relationships exactly. For example, modelers often use standard functional forms for convenience, such as linear or logarithmic equations, when the true relationship may not fit either of those functions perfectly. Model uncertainty can also arise from application of a model that was calibrated and validated for a different site, without sufficient recalibration and validation to adjust for local conditions. When simulating the effects of a remedy, data from a pilot study can provide a basis for recalibration using new initial conditions. This can reduce model uncertainty.

Input uncertainty is a second distinct component of uncertainty. Even if the selected model is correct in form, there may be errors in model parameters. For example, coefficients for partitioning between water and organic carbon can be obtained from handbooks of chemical parameters, and may be presented as ranges. A single value must be chosen, and the uncertainty in this parameter imparts an uncertainty to predicted partitioning and subsequent results. Model inputs, such as initial sediment contaminant concentrations and flows, are also subject to error, inherent with the instruments used to measure them and the reliability and consistency with which operators make those measurements. Finally, point estimates of concentrations and other inputs are averaged over model cells and treated as representing the entire cell uniformly. If cell resolution captures spatial trends well, then this aggregation error is of little consequence. If not, then it can be reduced by reducing cell size and taking enough samples to characterize each cell. However, such practices impart additional time and resource costs, and are justified only to the extent that the added detail helps inform the selection of a remedial alternative.

Even if the form of a model matches the physical phenomenon very well, parameters are calibrated closely, and inputs are measured with great accuracy, some *stochastic variability* will remain. This represents factors that cause actual values to be different from predictions and are not represented in the model. This may be because they are not well understood or because data have not been collected to explain them. The variability in fish tissue concentrations of contaminants is a good example. Much, but not all, of the variability in fish tissue concentrations can be explained by the species, age, length, lipid content, and sediment and water column contaminant concentrations. The rest of the variation may be due to natural variability between individual fish in habitat, diet, or genetic makeup. Models can predict average fish tissue concentrations for a given species as well as the range of natural variability around that average.

An understanding of all of the above sources of uncertainty is important for estimating and controlling the uncertainty in model predictions of present and future conditions. Model uncertainty can be reduced by going through the process of model development, hypothesis testing, and refinement described in the previous section on "What's in a model?" Uncertainty in inputs is translated into uncertainty in model outputs, and may be exaggerated or minimized depending on the sensitivity of the model to those inputs.

Model sensitivity is often measured by varying inputs by a fixed amount (commonly 10%) and observing the corresponding changes in key model outputs. This analysis helps users of models identify the key parameters driving the uncertainty in model predictions, and helps define where efforts to improve predictions are best placed (i.e., decreasing the uncertainty of the parameters to which the model is most sensitive).

Ultimately, the true "rightness" or "wrongness" (i.e., accuracy) of a model can never be known perfectly. But estimates of model uncertainty are possible, and can be helpful. The following section describes methods commonly used for quantifying model uncertainty, and some realistic expectations and limitations on the use of models.

How to Quantify Uncertainty

There are two distinct purposes to quantifying the uncertainty of a model. The first is to determine whether this model or an alternate model provides the better fit to the available data. The second is to estimate uncertainty bounds on predictions of the future.

To evaluate the goodness of fit to calibration data, measures of the typical deviation between predicted and actual values are usually used. These can be averages of deviations, or medians in cases where a few very large values might distort the average. Another common measure is the mean of squared deviations, called the root mean squared error. This measure is attractive because it is always positive and provides an estimate of the typical deviation in the same units as the variable itself (as opposed to those units squared.) As an intermediate step in model development, it is common to look at a set of these measures of typical model-data error and choose a candidate model formulation that performs best for the majority of the variables and goodness of fit metrics.

When a prediction is generated from a model, such as a time series of predicted future fish tissue concentrations, it is also important to estimate the upper and lower bounds of those estimates. In this example, the question may be whether bioaccumulation of the contaminant might be much lower or higher than the best estimate. This has traditionally been done in a number of ways: using parameter bracketing analyses; Monte Carlo analyses; by exploring alternative calibrations; and by making comparisons to validation data.

In a bracketing analysis, each key parameter of the model is selected and reset to the top and then to the bottom of its reasonable range, based on the judgment of the modeler. The two new forecasts that result bound the forecast, in terms of uncertainty in that parameter. For example, coefficients governing the adsorption of chemicals to organic carbon in sediment solids are measured in the laboratory, and handbook estimates may not be a perfect match to adsorption in the field. The type of carbon is also important: the amount of "black carbon" is usually unknown, and is a stronger adsorbent than other forms of carbon, tending to reduce contaminant bioavailability. A bracketing analysis shows how much this uncertainty matters, and how the forecast could differ with an adjustment in the value of this one uncertain parameter.

This procedure is sometimes extended to allow for simultaneous variation in multiple parameters. For example, a set of parameters could all be varied within reasonable ranges in a direction that lowers the series of predicted fish tissue concentrations to a lower bound, and then all varied in the opposite direction to generate upper bound predictions of future concentrations. This procedure is not recommended, because it generates best and worst cases that may be very unlikely and inconsistent with the data to which the model was calibrated, giving a distorted view of the spread between best and worst cases.

A preferred method is suggested by the calibration process itself. When a model has been well calibrated, and a parameter is then adjusted, the fit to data is worsened and compensating changes in another parameter or parameters are needed to restore a reasonable fit between model and data. The model is then run under a set of alternative calibrations, each perturbing one parameter from its calibrated value and then adjusting other parameters to produce a second-best model-data fit. The range of predictions generated by these alternative calibrations is consistent with the calibration dataset to nearly the same extent as the calibrated model, and should therefore be considered to be within reasonable uncertainty bounds. An exploration of the possibility of alternate calibrations of the model and an understanding of the range in outputs that can exist among these calibrations provides important insight into the uncertainty of model predictions.

A third technique for generating uncertainty bounds is Monte Carlo simulation. Named after the casino resort where dice are rolled and roulette wheels spun in games of chance, Monte Carlo requires the user to specify a distribution for each parameter to be varied, including correlations between parameters that are not considered to be independent. A series of forecasts is then generated, each one based on a draw of each parameter from its distribution of possible values. From this set of forecasts, a range of predictions of each variable at each future date is produced. The validity of this range depends on the validity of the assumed parameter distributions, including correlations between parameters. The modeler's experience that a change in one calibrated parameter must be offset by a change in another to restore goodness of fit suggests that parameters are typically correlated, and unless those correlations are known and specified, the output of a Monte Carlo simulation may overstate the spread between extreme predictions. This method is clearly only practical if multiple model runs can be generated in a short time, which is not the case for the most linked sediment/contaminant transport models.

Finally, an important check on the actual performance of a model is by comparing to a dataset independent of the data used to calibrate. A validation dataset provides a way to verify the accuracy of model predictions, identify unanticipated bias in important outputs, and test the validity of uncertainty estimates made using other methods.

Realistic Expectations and Limitations

An important objective of modeling is to make sound, reasonable predictions. A good calibration demonstrates that a model can do this, by simulating state variables accurately within the calibration period. No model can fit the data perfectly, however, for the reasons discussed above. For future periods, outside the calibration dataset, additional unknowns may come into play, so differences between actual and predicted values for future periods can be expected to be at least as great as those for the calibration period. This is why it is good practice to validate a model for a dataset that is held in reserve during calibration. The differences between actual and predicted values in calibration and validation provide the best indication of the size of the prediction errors that we can expect if we use the model to make short-term predictions.

For contaminated sediment sites, recovery may take decades, even with active remediation, so models are used to make very long term predictions under a variety of remedial alternatives. Observers of weather forecasts and economic forecasts know that uncertainty tends to increase as the period of the forecast is extended into the future (Figure 3). This increase in uncertainty is expected in environmental fate and transport forecasting for several reasons. For one thing, there may be unexpected changes in or shocks to the system that are not reflected in a model fit to current data. Examples are possible temperature or flow changes due to gradual global climate change, flow changes due to dam removal and/or urban development, or changes in background contaminant loads.

In addition, long-term sediment forecasts predict trends in state variables, and these can depend on predicted rates of long-term release or burial of the sediment inventory of contaminant. If those predicted rates are too high or too low, then absolute prediction errors in sediment, water column, and tissue concentrations tend to grow with time. For a good long-term forecast, the expectation should be that predicted *rates* of growth or decay in concentrations are accurate, while the absolute *magnitudes* of predicted concentrations are subject to increasing uncertainty over time. The more thoroughly a model has been calibrated and validated, using a data set spanning a number of years, and the more accurately remedies have been represented in the model, the more confidently those trends can be compared. Comparisons of the predicted absolute concentrations to target values are more uncertain, especially if they are the results of very long forecasts.

Forecasts of concentration trends under competing remedial alternatives are discussed in the next section.

Characterization of Uncertainty in Models

Both developers and users of models generally agree that all models are uncertain. Increasingly, modelers and project managers are moving beyond an acknowledgement of uncertainty to something more useful – a quantification of the degree of uncertainty in models, and estimation of its importance in model application. Quantified uncertainty is useful in designing sampling programs, in answering management questions that have “gray areas”, and especially in remedial decision making. The example below describes the development of a complex model, and a process by which the major sources of uncertainty in the model were identified, and impacts on the uncertainty in model output were quantified.

Example*:*

Background: At a riverine contaminated sediment site, an historical accumulation of sediments in depositional dam impoundments is now an ongoing source of contaminants to the river, due to removal of the dams and incising of the river into the former impoundment sediments. Because the river channel dropped, the river banks upstream of the former dams are now composed of contaminated sediments that act as a continuing source of solids and solids-associated contaminants to the river. (cont’d)

Model development: An EFDC model is constructed that represents the current distribution of contaminants in the river bed, banks, and former impoundment areas. Extensive data are available on historical trends in sediment and fish tissue contaminant levels. An important input to the model is an empirical analysis of the rate of bank erosion in the former dam impoundments, and the corresponding contribution of solids and contaminant load to the river. The river is also impacted by significant flow rate variation, with different mass transfer processes that operate under low flow conditions (contaminant diffusion from the bed) and high flow conditions (particle resuspension). The model is developed over several field seasons to provide a robust dataset and to account for all processes relevant to contaminant transport, producing a model that is well-calibrated and validated to sediment and contaminant data, capturing spatial variation in contaminant concentrations and trends in contaminant levels.

Uncertainty Analysis: Following model development, the modeling team and the project management team meet to post-analyze the model, trying to understand 1) what are the most important measures of model performance, and 2) what are the most important model inputs (processes and parameters) that affect those measures. As critical performance metrics for demonstrating model success, the group identifies a close correspondence of model predictions to:

- Field measurements of total suspended solids (TSS)
- Field measurements of dissolved, suspended and sediment PCB
- Site-specific burial rates indicated by geochronological studies
- Long-term recovery rates in sediment and fish

While many parameters and processes are identified as important, five are identified as critical for meeting the above performance metrics:

- Flow-dependent particle settling velocity
- Sediment resuspension rate coefficients
- Critical shear stresses for initiating bank erosion
- PCB mass transfer rate coefficients, for example the rate at which PCBs migrate from sediment pore water to overlying water due to diffusion or groundwater upwelling
- Bank erosion rates

In order to explore overall uncertainty in model predictions, the above coefficients are varied to explore the degree to which they impact model output. The allowable degree of variation in the above parameters is bounded on both the input and output sides of the model. On the input side, parameter variation is limited to the known uncertainty in the parameters (range of reasonableness), and on the output side, the degree to which parameter variation impacts the quality of the model calibration (calibration constraint). The effect of this range of variation on long-term forecasts of system recovery provides a useful, meaningful bound on prediction uncertainty.

HOW DO WE PREDICT REMEDIAL OUTCOMES?

Models are often used in Feasibility Studies to evaluate the short-term and long-term effectiveness of several alternatives. They can predict the time path of future exposures under each alternative, so that likely risk reduction can be estimated. Risk reduction is estimated relative to monitored natural recovery (MNR), which includes monitoring without active remediation. Calibration and validation of the model to pre-remedial data optimizes the representation of natural processes, which are relied upon by the MNR alternative. This section explains how an MNR forecast is developed, and how its initial conditions are modified to generate forecasts for active remedies. An MNR simulation is straightforward to develop, because it represents a continuation of natural conditions, and is a natural baseline scenario upon which to build active remedy scenarios. The development of updated bed conditions for representing the expected outcomes of active remedies using models and/or pilot studies also deserves considerable effort to minimize uncertainty. The use of MNR as a baseline for future scenario development does not reflect any presumption, in favor of MNR or any other remedy.

From Validation to Prediction - Monitored Natural Recovery Forecasts

Contaminated sediment model simulations begin with initial conditions of sediment concentrations, add external forcings including flows and temperatures, and generate time series of predicted concentrations for media of concern. During model development this is done for calibration and validation periods, which often coincide with the period of the remedial investigation (Figure 3).

For remedial planning, forecasting is extended into the future. The calibration or validation runs can be continued beyond the remedial investigation period into the future, or the simulation can be restarted if current sediment concentrations are available to reset initial conditions. Future flows and other weather-related forcings are unknown, but can generally be expected to follow patterns similar to past data unless major system changes have occurred (*e.g.*, changes in dam operations, watershed development). To simulate future years, past time series can be recycled through the forecast period.

The result of the MNR simulation is a forecast of surface sediment, water column, and tissue concentrations. This forecast is our best estimate of potential future exposures, under an MNR remedy. To translate these predicted exposures into time series of expected human health and ecological risks, risk factors developed in the baseline risk assessment can be applied. The objective of protection of human health and the environment amounts to reducing this series of current and future risks.

The Role of Solids in Forecasts

Solids play a key role in chemical fate and transport at contaminated sediment sites, and physical and chemical processes involving solids have been emphasized throughout the discussion above. We revisit those processes to discuss a critical element of forecasting, namely how models simulate the adsorbed concentrations of chemicals on solids. Regardless of the remedy selected, solids accumulation is likely to occur in portions of the remediated area, and the concentrations of contaminant on those solids will be a major driver of post-remedial exposure and risk. Indeed, with both MNR and more active remedies, the simulated time trend of those concentrations can determine the expected time to achieve remedial goals.

Contaminant concentrations on fresh solids deposits are determined as follows. Some of the solids that move down a river in suspension are present because of upstream erosion. Solids are deposited at lower flows and eroded at higher flows, and net accumulation or depletion of solids depends on which flows predominate. Models simulate a depth of erosion as a function of flow, flow history, and sediment physical properties (i.e. is sediment fresh and fluffy or older and more compacted), and ideally do so using data (where sediments are cohesive) from flume studies using site-specific sediment samples (p. 19). These solids are then tracked by models as suspended in the water column or settled at downstream locations, as stream velocities decline with time or at a widening of the channel cross-section.

Along with eroded solids, additional solids enter waterbodies from upstream, from tributaries and shoreline erosion. Those loads can be strongly related to flow, and the relationship between flow and tributary loads can be determined by monitoring or by watershed modeling, using land-use and rainfall data. Solids loads from smaller tributaries that are not monitored or modeled can be estimated as proportional to similar subwatersheds, scaled according to ratios of the subwatershed areas. It should be emphasized that accounting for watershed solids is critical to simulating long-term system behavior, because long-term changes in the sediment surface depend on solids in minus solids out of the system.

Suspended solids are a mix of contaminated material from eroded deposits and watershed solids, which are typically less contaminated (one notable exception being the potential input of contaminated solids from storm drain outfalls). Models simulate the mixing of those solids to produce an average concentration of contaminant on solid particles. At the same time, models simulate some contaminant desorption from solids into surface water, or adsorption in the opposite direction, according to an equilibrium partitioning relationship that typically leaves most of the contaminant associated with the solids. Models then simulate settling such that it is greatest at the lowest stream velocities.

This is how models simulate concentrations and deposition rates of freshly deposited sediment. If erosion is primarily from the top layer of sediments, then the newly deposited surface sediments will have some contamination, but possibly at reduced levels because of dilution by cleaner watershed solids. Under extreme conditions, if sediments are eroded deeply into buried legacy contamination, surface concentrations could be increased, in spite of dilution by watershed solids.

Forecasts of Alternative Remedies

To assess the long-term risk reduction benefits of alternative remedies, parallel forecasts can be generated and translated into alternative risk forecasts. These are similar to the MNR forecast, using the same forcing functions and calibrated model parameters, but with updated bed conditions incorporating the expected effect of the remedy on baseline conditions. The long-term natural processes of burial, mixing, and dilution by watershed sediments can enhance the effectiveness of active remedies, and model simulations forecast the extent to which that would be expected to occur.

How to Specify Post-remedial Conditions

One critical aspect of the active remedial simulations in a Feasibility Study is that updated bed conditions must be assumed rather than measured, because the remedy has not yet taken place (and most of the simulated alternatives will not be implemented.) This adds an additional layer of uncertainty that is not present in the MNR forecast. These starting conditions for remedial simulations are not generated by the contaminant transport model; they are computed offline based on knowledge of the remediation technology and site conditions. In addition, the updated bed characteristics that are specified may be outside of the range of conditions to which the model has been calibrated and validated.

To minimize this additional uncertainty, assumptions about modified bed conditions should use the best available quantitative tools. Available tools are discussed below. In general, the performance of the remedy should be modeled based on a thorough synthesis of pilot performance at the site and the performance of remedies at other sites with similar conditions.

For example, engineered caps and post-dredging residual covers can be expected to change site conditions in these ways:

- reduced surface sediment contaminant concentration
- coarser surface (sand or gravel)
- reduced organic carbon content, and
- reduced water depth.

The coarseness of the surface material is usually by design, to resist erosion and increase physical stability of the sediment bed. Modeling of the shear stresses to which caps will be subjected under high flows is commonly done as part of remedial design. Modeling of short- and long-term risk reduction due to capping also helps in evaluating the potential benefits of this option.

Sands and gravels have higher permeabilities and lower carbon content than native silts and clays, increasing the potential for movement of contaminated pore water into clean cap materials. Contaminant movement, if likely to present a problem, can be addressed in several ways during cap design, including by adding materials with greater organic carbon or other sorbent to the cap. The modeling of pore water transport through the cap can be performed using a satellite model specifically designed for this purpose (Palermo *et al*, 1998, Reible and Marquette, 2009).

Unless placed in combination with dredging, caps also reduce water depth, thereby reducing the channel cross-section. By incorporating these bathymetric changes in a hydrodynamic model, any resulting increases in stream velocity and/or flooding can be predicted.

The following conditions can be expected to result from environmental dredging:

- removal of sediment to a target depth
- some generated residuals left in place
- resuspension of sediment to the water column, containing adsorbed contaminant
- release of dissolved contaminant to the water column via desorption from sediment or pore water release
- some undredged inventory left in place, and
- a sand cover or backfill, when specified as part of the design.

The extent to which generated residuals are left in place will depend on the concentrations of the material being dredged, the difficulty of removing it cleanly (as may be affected by debris or underlying bedrock), and the limits of the dredging technology (NRC 2007b, Bridges *et al*., 2008). Some undredged inventory may also be left in place, depending on the completeness of sediment characterization and the tolerance of the post-construction monitoring program.

The expected extent and vertical distributions of these post-dredging inventories, based on knowledge of pre-remedial deposits and experience at sites with similar conditions and dredging techniques, should be estimated and used as updated bed conditions. A practical approach to estimating residual concentrations a priori, based on experience at other sites, is outlined in Palermo *et al*. (2008).

This is important information for sound remedial planning, whether or not models are used to support that planning. The more realistic and better informed the assumed bed conditions in remedial forecasts, the more likely that the long-term consequences of the remedy can be reliably predicted.

Similarly, updated bed conditions must be assigned when sand covers, engineered caps, reactive caps, or other remedial technologies are simulated. Formulating updated bed conditions for sand cover and capping alternatives is more straightforward than for dredging, because the resistance of sands, gravels, and stone of given diameters is well known, as are their contaminant concentrations. Nevertheless, their placement can cause mixing with soft sediment, and ideal placement should not be assumed without justification. Pilot studies of remedial technologies can provide very valuable information for setting updated bed conditions, thereby reducing uncertainty in forecasts under remedial alternatives.

Some release of contaminant to the water column is also expected during remediation, and the resulting short-term exposures and contaminant export can have an effect on bioaccumulation and risk. Estimates of contaminant loss during dredging range from less than 1% to up to 9% of contaminant mass dredged, and will depend on sediment properties, vertical contaminant distribution, dredging methods, and salinity (EPA 2005). Releases to the water column can be evaluated through a pilot dredging study or from experience at sites with similar characteristics and remedial technologies.

How to Model Extreme Events and Evaluate Long-term Effectiveness

Long-term effectiveness is an essential component of any contaminated sediment remedy. This is assessed by evaluating each remedy under conditions of high erosive shear stress, which could occur due to an extreme flow event, wind waves, or tidal surges (which have a close counterpart in fresh water bodies in the form of seiches.)

These extreme events should be considered in the Feasibility Study evaluation of long-term effectiveness and permanence of the remedy as well as in the remedial design. It is likely that the most extreme events measured in the calibration and validation data sets fall short of the extremes expected over the lifetime of the remedy. It is common to consider the effects of a flow event expected to occur once every 100 years, on average, and other extreme events having similar recurrence intervals.

Such an event can be inserted into a long-term forecast to assess its effect on exposure and risk. The hydrodynamic model simulates local stream velocities for the event and resulting shear stresses on the bed. Where native material is left in place, as in MNR, the site-specific erodibility relationship that is already built into the model can be used to predict the depth of erosion and resulting release of contaminant. Where specific sizes of sand or gravel are placed on the bed for capping or for a post-dredging residual cover, the modeler can consult the widely published “Shields Curve” to obtain the shear stress needed to cause erosion.

The consequences of an extreme event are likely to be greater for post-MNR than for post-dredging, because of smaller inventories of buried contaminant in most post-dredging scenarios. Simulated effects of extreme events on caps and covers depend primarily on their thickness, selected grain sizes, and erosive forces. Simulations of their permanence under extreme events can be an aid to conceptual design, supporting estimates of the cost to provide sufficient protectiveness.

Comparisons of Risk Reduction Under Competing Alternatives

With parallel simulations of possible remedies in place, the predicted outcomes can be compared. These take the form of time lines of exposures and resulting risks. In making this comparison, differences in time to plan and implement the different remedial alternatives should be taken into account, because these project phases can take many years for active remedies at large sites. When compared to MNR, some remedies may show long-term gains offsetting short-term setbacks. This can be the case, for example, where the alternative involves dredging high concentrations of buried sediment using technologies that release contaminants and leave some generated residuals in place, thereby at least temporarily increasing surface sediment and fish tissue contaminant concentrations. In such cases, the assessment of expected future risk should take both the short- and long-term effects into account, weighing a temporary increase in risk against a long-term reduction. At large sites, it may also be useful to model the short-term and long-term effects of combination remedies by varying the proportions and locations of MNR, capping, and dredging.

A comparison of the simulations of the various alternatives in the context of the National Contingency Plan criteria can support the selection of a remedy for the site. Comparisons for the various remedies of predicted contaminant concentrations in surficial sediments, the water column, and fish tissue represent expected differences in future contaminant exposure and risk. As suggested in the discussion of uncertainty above, absolute concentrations and risk levels predicted for the alternatives are subject to significant uncertainty on time scales of decades. Nevertheless, a comparison of model-predicted trends in risk under the available alternatives provides a useful means of quantifying overall risk reduction. Using process-based numerical models to do this ensures that decision-making is consistent with our best understanding of site data and long-term processes acting to increase or decrease exposures over time.

Simulations of the selected remedy are also a valuable asset when it comes time to monitor the effectiveness of the remedy. Model simulations set expectations for post-remedial time trends in concentrations and body burdens, as they are expected to vary from one location to another across the site. In this way model simulations can help in designing a monitoring plan, and also in informing the 5-year reviews of remedy protectiveness. Where recovery is faster or slower than expected, models can be recalibrated to the monitoring data, and if warranted, used to amend the selected remedy. From the initiation of the investigation to the completion of the remedy, process-based numerical models can help to test and refine our understanding of site contamination and the development of a cost-effective solution that achieves long-term protection while minimizing short-term adverse impacts.

Contact Information

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Using Models to Predict Remedy Effectiveness

A key function of a well-developed model is to aid in assessing the effectiveness of different remedy alternatives. Rather than choosing between a single major remedy implementation method (dredging, capping, MNR), models are often used to support evaluation of different combinations of remedies. At this point in the FS process, models provide input into economics of remedial alternatives, helping to find the best combination of remedy effectiveness and cost control. The example below describes how a model can be used to evaluate a typical combination remedy.

Example:

Background: At a riverine discharge into a coastal zone, historical data on PAH contamination show generally recovering sediments with some zones of persistent elevated contaminant concentration. Because of the effects of progressive urbanization of the watershed and changing hydrology, some of these areas have been identified as vulnerable to erosion under future extreme events.

Model Development: Based on the historical record of PAH data, academic studies of sediment loads to the river, and several phases of RI investigation, an EFDC model is used to document recovery of surficial sediments. The model is well calibrated, based on reach-based estimates of deposition and burial, plus site-specific bioturbation rate measurements that constrain surficial mixing and dilution. The model is developed to a resolution sufficient to capture remedy implementation at the 100-foot scale. Building on the exposure fields generated with the EFDC model results, a Gobas model is developed and calibrated to fish body burdens.

Remedy Representation: The proposed remedies include combinations of MNR, capping, and localized “hot spot” dredging. A key role of the model is to identify the relative benefits of different combinations of the remedial alternatives.

Model implementation procedures:

MNR: The process of model development and testing build strong stakeholder acceptance of the model’s ability to represent the bioturbation, deposition and burial processes that affect the viability of MNR. Incorporation of changing hydrology due to watershed development indicates that recovery processes are expected to continue well into the future, but also directs attention to a few areas of elevated contaminant levels and potential for exposure under extreme event conditions.

Capping*:* Areas of potential vulnerability to future erosion are addressed with a capping remedy. The remedy is represented in the model by zeroing out resuspension in affected model cells. Transport through the cap is limited to slow diffusion through the cap, which is simulated with a simplified offline submodel. Based on the findings of the submodel, diffusion through the cap is judged to be insignificant and is zeroed out in the EFDC model.

Dredging*:* In a few areas of significantly elevated concentrations, dredging is recommended to meet stakeholder objectives for risk management. The remedy is implemented in the model by assuming a clean sand backfill (background concentrations).

Habitat creation*:* The remedy also addresses the impact of habitat limitations on the fish population. Habitat creation is focused on areas of high restoration potential that coincide with very low contaminant levels. In the Gobas model, habitat preference factors for fish are modified to favor newly created habitat areas in remediated areas.

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APPENDIX A: A Partial Listing of Available Hydrodynamic, Sediment Transport, Contaminant Transport, and Food Chain / Ecological Effects Models

Hydraulic/Hydrodynamic/Sediment Transport/Contaminant Transport Models

CE-QUAL-W	USACE Dynamic, 2D Laterally-Averaged Water Quality Model
CH3D-SED	USACE Dynamic, 3-D Curvilinear Hydrodynamics and Sediment Transport Model
CORMIX	USEPA 3-D Steady-State Analytical Mixing-Zone Model
DYNHYD5	USEPA/CEAM Dynamic 1-D Link-Node Tidal Hydrodynamic Model
ECOMSED	HQI Dynamic, 3-D Hydrodynamic and Sediment Transport Model
EFDC	Tt/VIMS/EPA 3-D Environmental Fluid Dynamics Code
HEC-RAS	USACE Dynamic, 1-D River Analysis System
HEM1-3D	VIMS Dynamic, 1-3D Hydrodynamic and Eutrophication Models
HSCTM-2D	USEPA/CEAM 2-D Dynamic Hydrodynamic Sediment and Contaminant Transport Model
RCA	HQI Dynamic Water Quality Simulation Model
RIVMOD-H	USEPA/CEAM Dynamic, 3-D River Hydrodynamic Model
RMA-2V	WES Dynamic, 2-D Hydrodynamic Analysis Model
WASP5/6/7	USEPA Dynamic Water Quality Simulation Model

Hydrologic/Watershed Models

AGNPS	USDA Agricultural Non-Point Source Pollution Model
BASINS	USEPA/CEAM Point and Non-Point Source Model Toolbox
HSPF	USEPA/CEAM Simulation of Mixed Land-use Watersheds
SWAT	USDA Soil and Water Assessment Tool
SWMM	USEPA Stormwater Management Model
WARMF	EPRI Watershed Analysis Risk Management Framework

Food Chain / Ecological Effects Models

AQUATOX	USEPA Ecosystem / Food Web Bioaccumulation Model
AQUAWEB	Arnot and Gobas Food Web Bioaccumulation Model
BASS	Bioaccumulation and Aquatic System Simulator
ECOFATE	Gobas (1993) Model of Ecological Fate and Food Web Bioaccumulation
EXAMS II	USEPA/CEAM Fate and Exposure Model for Assessing Toxics

FGETS	USEPA/CEAM Food and Gill Exchange of Toxic Substances Fish Bioaccumulation Model
HEP/HS	USEPA/CEAM Habitat Evaluation Procedures/Habitat Suitability Indices
HES	USEPA/CEAM Habitat Evaluation System Used to Assess the Impacts of Development Projects for Aquatic and Terrestrial Habitat Evaluations
IFIM	USEPA/CEAM Instream Flow Incremental Methodology for Riverine Habitats
PHABSIM	USEPA/CEAM Fish-habitat Preference and Discharge-Habitat Model
PVA	USEPA/CEAM Population Viability Analyses
QEAFDCHN	QEA Food Chain Bioaccumulation Model
RBPs	USEPA/CEAM Rapid Bioassessment Protocols
SERAFM	Spreadsheet-Based Ecological Risk Assessment for the Fate of Mercury
THOMANN	Thomann Fish / Food Web Model