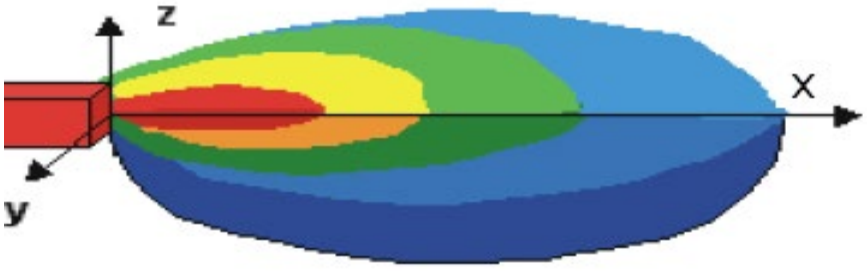
State of Ohio
Environmental Protection Agency

Division of Drinking and Ground Waters

Technical Guidance Manual for Ground Water Investigations

Chapter 14

Ground Water Flow and Fate and Transport Modeling



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TECHNICAL GUIDANCE
MANUAL FOR
GROUND WATER INVESTIGATIONS

CHAPTER 14

Ground Water Flow and Fate and Transport Modeling

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PREFACE

This document is part of a series of chapters incorporated in Ohio EPA's *Technical Guidance Manual for Hydrogeologic Investigations and Ground Water Monitoring* (TGM), which was originally published in 1995. DDAGW now maintains this technical guidance as a series of chapters rather than as an individual manual. These chapters can be obtained at http://www.epa.state.oh.us/ddagw/tgmweb.aspx.

The TGM identifies technical considerations for performing hydrogeologic investigations and ground water monitoring at potential or known ground water pollution sources. The purpose of the guidance is to enhance consistency within the Agency and inform the regulated community of the Agency's technical recommendations and the basis for them. In Ohio, the authority over pollution sources is shared among various Ohio EPA divisions, including the Emergency and Remedial Response (DERR), Hazardous Waste Management (DHWM), Solid and Infectious Waste (DSIWM), and Surface Water (DSW), as well as other state and local agencies. DDAGW provides technical support to these divisions.

Ohio EPA utilizes ***guidance*** to aid regulators and the regulated community in meeting laws, rules, regulations, and policy. Guidance outlines recommended practices and explains their rationale. The Agency may not require an entity to follow methods recommended by this or any other guidance document. It may, however, require an entity to demonstrate that an alternate method produces data and information that meet the pertinent requirements. The procedures used usually should be tailored to the specific needs and circumstances of the individual site, project, and applicable regulatory program, and should not comprise a rigid step-by-step approach that is utilized in all situations.

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TECHNICAL CHANGES FROM THE FEBRUARY 1995 TGM

The Ohio EPA Technical Guidance Manual for Hydrogeologic Investigations and Ground Water Monitoring (TGM) was finalized in 1995. This guidance document represents an update to Chapter 14(Ground Water Modeling). Listed below are the major technical changes from 1995.

1. Additional introductory language, including more detailed discussion on types of models that may be used at Ohio EPA regulated sites has been added.

2. Web sources are provided that may aid in model selection.

3. Some common input parameters were identified. Information is provided on whether the inputs should be based on site-specific data collection or whether there are any acceptable default values (Appendix A).

CHAPTER 14

GROUND WATER FLOW AND FATE AND TRANSPORT MODELING

Ground water flow and contaminant fate and transport models are used to help understand and evaluate hydrogeologic systems. Models are simplified representations or approximations of real hydrogeologic systems and may incorporate a number of processes operating within ground water and/or unsaturated zones. The purpose of modeling can vary widely, and the approach used may depend on site-specific needs, current understanding of the hydrogeologic system, availability of input data, and expectation and use of the model results. Models are typically used to:

- Evaluate ground water movement, flow direction, velocity, and discharge rates.
- Evaluate the interaction between hydrogeologic systems.
- Interpolate between known measurement points.
- Identify data gaps during site characterization.
- Aid in the development and management of ground water supply systems.
- Simulate changes in flow conditions resulting from stresses to a ground water zone.
- Determine potential impacts of contamination to nearby wells or surface water.
- Aid in the design and/or performance of remedial systems.
- Estimate leachability from soil sources to ground water.
- Demonstrate compliance with regulatory requirements.
- Estimate vapor intrusion from ground water and soils into buildings.
- Estimate capture zones and drinking water source protection areas.

Models are not a substitute for field investigations, but should be used as supplementary tools. They produce estimates, not a absolute answers. Results depend on the quality and quantity of the field data available to define input parameters and boundary conditions (Wang and Anderson, 1982). Results should always be evaluated in context with the fundamental assumptions of the model and the adequacy of the input data. Modeling may be of limited value when: a remedy can be readily identified, available data indicate there is not an environmental problem, or the site is too complex to model realistically. If a site is poorly characterized or poorly understood, any simulation of the transport and impacts of contaminants using models could be misleading. The use of models under such circumstances can help to support only limited types of decisions, such as planning and prioritizing activities. As a general rule, it is prudent to continually question the results of modeling and the potential consequences of decisions based on misleading results, and consider what can be done to verify results (U.S. EPA, 1996c).

Because major decisions frequently are based on modeling results, it is essential that modeling be conducted in a manner that provides confidence that the results portray field conditions. Thus, the effort must be documented in detail. This chapter identifies types and uses of models and the necessary documentation. It is not intended to provide approval/authorization for particular models. Internet addresses are provided that discuss various public domain and, in some cases, proprietary models. This does not represent an Ohio EPA endorsement of any model.

GROUND WATER FLOW MODELS

Ground water flow models are used to simulate the rate and direction of movement through the subsurface. This simulation requires a thorough understanding of the hydrogeologic system. Hydrogeologic investigations should include a complete characterization of:

- Subsurface extent and thickness of aquifers and confining units (hydrogeologic framework).
- Hydrologic boundaries (also referred to as boundary conditions), that control flow.
- Hydraulic properties of the ground water zone and confining units.
- Horizontal and vertical distribution of hydraulic head throughout the modeled area for beginning (initial conditions), equilibrium (steady-state conditions) and transitional conditions when hydraulic head may vary with time (transient conditions).
- Distribution and magnitude of groundwater recharge, pumping or injection of ground water, leakage to or from surface-water bodies, etc. (sources or sinks, also referred to as stresses). These stresses conditions may be constant or transient.

The outputs from model simulations are the hydraulic heads and groundwater flow rates, which are in equilibrium with hydrogeologic conditions (framework, boundaries, initial and transient conditions, hydraulic properties, and sources or sinks) for the modeled area. Models can also be used to simulate possible future changes to hydraulic head or ground water flow rates as a result of future changes in stresses on a ground water zone.

FATE AND TRANSPORT MODELS

Fate and transport models simulate the movement and chemical alteration of contaminants as they move through the subsurface. They may be used to model contaminants in both the ground water and vadose (unsaturated) zone.

Fate and transport models used to model transport within a ground water zone require the development of a calibrated flow model or, at a minimum, an accurate determination of the flow velocity, which has been based on field data. The model simulates the following:

- Movement of contaminants by advection, diffusion, and dispersion.
- Removal or release of contaminants by sorption or desorption from soil or rock.
- Alteration of contaminants by biological or physical processes, or by chemical reactions.

In addition to a thorough hydrogeological investigation, the simulation of fate and transport processes may require characterization of:

- Horizontal and vertical distribution of average linear ground water velocity (direction and magnitude) determined by a calibrated flow model or through accurate determination from field data.

- Initial distribution of solute.
- Location, history and mass loading rate of chemical sources or sinks.
- Effective porosity.
- Soil bulk density.
- Cation exchange capacity.
- Fraction of organic carbon in soils.
- Octanol-water partition coefficient for chemicals of concern.
- Density and viscosity of non-aqueous fluid.
- Longitudinal and transverse dispersivity.
- Diffusion coefficient.
- Chemical decay rate or degradation constant.
- Equations describing chemical transformation processes, if applicable.
- Initial distribution of electron acceptors, if applicable.

The outputs from model simulations are contaminant concentrations that are in equilibrium with the groundwater flow system and geochemical conditions (described above) for the modeled area.

As with flow models, fate and transport models should be calibrated and verified by adjusting values of the different hydrogeologic or geochemical properties to reduce any disparity between the simulations and field data. This process may result in a re-evaluation of the model used for simulating flow if the adjustment of values of geochemical data does not result in an acceptable simulation. Predictive simulations may be made with a fate and transport model to predict the expected concentrations of contaminants as a result of implementation of a remedial action. Monitoring of hydraulic heads and groundwater chemistry may be required to support predictive simulations.

TYPES OF MODELS

Models use a single equation or a set of governing equations that represent the process(es) occurring (e.g., ground water flow, solute transport, etc.). They can be analytical or numerical; deterministic or stochastic; or steady state or transient. In addition, models can be one-, two-, or three-dimensional. The various types are discussed below. Table 14.1 provides guidance on one-, two-, and three-dimensional models.

Table 14.1 Use of One-, Two-, and Three-Dimensional Models.

DIMENSION	USES
One-Dimensional	• Initial assessments where the degree of the ground water zone heterogeneity or anisotropy is not known. • Sites where a potential receptor is immediately downgradient of a contaminant source. • Model inputs are conservative.
Two-Dimensional	• Problems that include one or more ground water sources/sinks (e.g. pumping or injection wells, drains, rivers, etc.). • Sites where the direction of ground water flow is obviously in two dimensions (e.g. radial flow to a well or single ground water zone with relatively small vertical hydraulic head or contaminant concentration gradients). • Sites at which the ground water zone has distinct variations in hydraulic properties. • Contaminant migration problems where the impacts of transverse dispersion are important and the lateral, or vertical, spread of the contaminant plume must be approximated. • Large ratio between horizontal length and ground water zone thickness. • Thin ground water zones. • Model inputs are conservative.
Three-Dimensional	• The hydrogeologic conditions are well known. • Multiple ground water zones are present. • The vertical movement of ground water or contaminants is important. • Large vertical components exist (e.g., near springs, rivers). • Objectives require detail modeling. Extremely detailed and accurate results that closely match site conditions are needed.

ANALYTICAL MODEL

Analytical models are based on exact solutions to one- or two-dimensional ground water flow or transport equations. These equations are simplifications of more complex three-dimensional ground water flow and solute transport equations used in numerical modeling. Analytical models require a simplification of the flow system, including a horizontal aquifer base, uniform hydraulic and chemical reaction properties, and simple flow or chemical reaction boundaries. In addition, analytical models are typically steady-state and one-dimensional, although selected ground water flow models are two-dimensional (e.g. analytical element models) and some contaminant transport models assume one-dimensional ground

water flow conditions and one-, two- or three-dimensional transport conditions. Analytical models are best used:

- When designing data collection plans prior to beginning field activities.
- As an independent check of numerical model results.
- When field conditions support the simplifying assumptions embedded in the model.
- When field data shows that flow or transport processes are relatively simple.
- As an initial assessment of conditions or screening of remedial alternatives is needed.

Analytic element models (AEMs) have been developed that are capable of solving more complex regional flow problems through the superposition of hundreds of individual analytical solutions (or analytic elements) within one model. These analytic elements can represent complexities such as hydraulic conductivity inhomogeneities, streams, lakes, wells, variable recharge areas, etc. Another feature of AEMs is their lack of a model grid, which allows the user to extend the model indefinitely to incorporate regional features without sacrificing accuracy in the area of interest. For more information, see *Analytic Element Modeling of Groundwater Flow* (Haitjema, H.M. 1995).

NUMERICAL MODELS

Numerical models (e.g., finite difference or finite element) solve the partial differential flow or solute transport equations through numerical approximations using matrix algebra and discretization of the modeled domain. In discretization, the model domain is represented by a network of grid cells or elements and the time of the simulation is presented by time steps. The accuracy of numerical models depends on the model input data, the size of the space and time discretizations, and the numerical method used to solve the model equations.

Where the ground water system is very complex, and where sufficient data exist to simulate the complexities in detail, a numerical model may be able to simulate the system with greater accuracy. Generally, they can model irregular boundaries, variations in input parameters such as hydraulic conductivity and recharge, vertical flow gradients at recharge and discharge areas, transient flow conditions, complex multilayered hydrogeologic framework, and other complexities.

Numerical models are best used when:

- Field data shows that ground water flow or transport processes are relatively complex.
- Ground water flow direction, hydrogeologic or geochemical conditions, and hydraulic or chemical sources are sinks that vary with time and space.
- Appropriate input data is available for the model.

Numerical models may be of limited value when there are limited data and in simple hydrogeologic settings where the cost of creating such a model outweighs the information.

DETERMINISTIC VERSUS STOCHASTIC

Most computer models utilize a deterministic approach where all data are input as single, "best estimate" values. Single value inputs result in single value outputs. When modeling on a site-specific scale, where extensive data has been collected and spatial characterization is well established, a deterministic approach is generally appropriate. Simulations with appropriate calibration, sensitivity analysis, and history matching can produce an adequate representation of the real hydrogeologic system. If the modeling effort utilizes very limited data or where a larger, regional scale is involved, a stochastic (statistical) approach may be acceptable (e.g., Monte Carlo simulations). This approach utilizes hydraulic parameters having a probability distribution that results in all output having the same probability distribution. A stochastic approach to modeling would characterize parameter uncertainty by incorporating a measure of uncertainty into the parameters and database utilized in the simulations.

When a lack of data and a high degree of data uncertainty exists, calibration and additional history matching can be long, tedious, or impossible. The stochastic approach allows the uncertainty factor to be maintained throughout the modeling process, allowing for potentially more realistic interpretations of the results by providing ranges of scenarios applicable to the real system. Too often, the data uncertainty factor is lost when deterministic approaches are utilized at sites for which limited data are available. The results become "fact" without acknowledgment of the limitations dictated by the input parameters and the underlying assumptions.

SIMULATION-OPTIMIZATION

Simulation-optimization couples mathematical optimization algorithms with ground water flow or contaminant transport models to determine the optimal solution when many solutions exist. It may help identify pumping solutions that:

- Minimize life-cycle cost, annual cost, or cleanup time while assuring protectiveness.
- Maximize mass removal.
- Minimize pumping rate required for plume capture.

There are two general subclasses of simulation-optimization, hydraulic optimization and transport optimization. Hydraulic optimization is based on ground water flow modeling and is used when containment is the primary concern. Transport optimization is based on both ground water flow and transport modeling and is appropriate when ground water restoration is the primary concern. Additional information can be found at the Federal Remediation Technology Web Site and U.S. EPA, 2004.

STEADY STATE VERSUS TRANSIENT

Ground water flow and fate and transport models simulate either steady state or transient flow. In steady-state systems, inputs and outputs are in equilibrium so that there is no net change in the system with time. In transient simulations, the inputs and outputs are not in equilibrium so there is a net change in the system with time. Steady state models provide average, long-term results. Transient models should be used when the ground water regime varies over time.

GENERAL PROTOCOL

The following paragraphs outline the general protocol that should be used to ensure that modeling is conducted and documented appropriately.

DEFINE THE PURPOSE/OBJECTIVES

The purpose/objectives of modeling should be clearly defined and understood because it dictates the selection and development of the model. Additional factors that should be considered are regulatory requirements, potential risk to human health and the environment, site complexity, and economic constraints.

Note that models are tools only and are not a substitute for field data. For example, an evaluation of the effectiveness of a proposed ground water remedial system may be based on modeling. However, a verification that the existing remedial system is adequately cleaning up the ground water needs to be based on field data.

QUALITY ASSURANCE PLANS

Quality assurance is a component of site investigations to ensure that data collection and interpretations have been appropriate. Quality assurance may need to be considered during the development, application, and verification. Development of a quality assurance plan at the beginning of modeling will help ensure more reliable results. The following may need to be addressed (California EPA, 1995):

- Protocols for field data collection, verification, and processing.
- Narrative and graphical presentation of a conceptual model, including description of processes to be considered.
- Criteria for model selection.
- Documentation and retesting when changes are made to a model code.
- Protocols to be followed in model formulation.
- Protocols to be followed in model calibration, including, limits on parameter adjustments, and identification of calibration goals.
- Protocols for sensitivity analysis.
- Procedures for analysis of error.
- Level of information to be included in computer output.
- Applicability of the specific modeling program and mathematical formulas.
- Assumptions made and their potential influence on model output.

- Establishment of record keeping procedures to document the model application process.

- Format for presentation of results.

CONCEPTUAL MODEL DEVELOPMENT

A conceptual model should be developed. This is critical in any modeling project (Bear et al., 1992). A conceptual model is a simplified description and schematic that outlines the components of the system to be modeled. The model must be based on a thorough understanding of site hydrogeologic conditions derived from field investigations and regional data obtained from academic or government studies (see Chapter 3). At a minimum, the conceptual model should include the geologic and hydrologic framework, hydraulic properties, areas of recharge and discharge (sources and sinks), boundary and initial conditions, transport processes, and spatial and temporal dimensionality (U.S. EPA 1996a & b). For contaminant transport modeling, additional factors should be incorporated, including (but not limited to), contaminant sources when released (if known), media affected, and concentration distributions. In addition, the physical and chemical properties of the contaminants that may affect their movement should be evaluated. Conceptual models should be continually refined as more data are obtained. ASTM E1689 provides additional guidance on the development of a conceptual model. (Note: the ASTM guidance is for a *site conceptual model* for all pathways, not just ground water.)

MODEL SELECTION

A model should be chosen based on its applicability to the conceptual model, availability of the required input data, and the defined purpose/objective of the modeling effort. It is important to choose a model that simulates the natural system as accurately as possible. The model should satisfy fundamental assumptions and the boundary and initial conditions of the area to be modeled. The user will need to decide whether it is more appropriate to use an analytical model versus numerical and also whether to use a one-, two- or three dimensional model (See section on Types of Models, page 14-4). In addition, it is important that any model selected be code-verified, peer-reviewed, and documented.

- **Code verification** is a process of checking the accuracy of the algorithms used to solve the governing equations, thereby demonstrating that the model actually approximates the process equations for which it is being applied. This can be accomplished by solving a problem with the model and comparing the results to those obtained from an analytical solution or to another model that has been verified. *(Note: Code verification does not ensure that the model can solve important problems, or correctly reflects the real world process.*)

  The publication of a model or its availability for sale does not necessarily mean that the model has been code-verified. If the model has been code-verified in the literature or user's manual, evidence of this information can be used to document that the model has been verified. The results of the code-verification should be included in reports summarizing the model results.

- It is important that the chosen model has been **peer-reviewed**. Modelers often choose to employ a general but widely used model rather than one that is specialized

and less well known because the widely used model's code has been widely tested in numerous settings and should be relatively free of "bugs."

- The model should be well **documented.** The fundamental assumptions and limitations of the model, the mathematical solution techniques, and the code structure should be documented. In addition, documentation should include instructions on how to use the model, input data requirements, and an explanation of the output. ASTM D6171-97(2004) provides additional information on documenting a ground water modeling code.

Contaminant transport modeling should include simulation of advective flow, which is typically the major component of contaminant transport. Mechanical dispersion and diffusion also can play a role, and these parameters are often lumped into a single dispersion value (Faust and Mercer, 1980). Sorption and transformation processes (e.g. biodegradation, hydrolysis, etc.) can change the physical or chemical state of contaminant(s). When modeling contaminant movement, all applicable transport processes should be considered. Excluding or combining any of the processes must be justifiable.

The following Web sites may aid in the selection of a model.

International Ground Water Modeling Center, Colorado School of Mines (IGWMC).
Can purchase models and download demos or free software. Provide technical support.

Ground Water and Ecosystem Restoration Research. U.S. Environmental Protection Agency. (Formerly Kerr Labs: Center for Subsurface Modeling Support (CSMoS)). Access to EPA public domain models and other technical support information.

NTIS, National Technical Information Service. Source for the sale of scientific, technical and engineering products produced by or for the U.S. government.

U.S. Geological Survey. The software and related documentation on these Web pages were developed by the U.S. Geological Survey (USGS) for use by the USGS in fulfilling its mission. The software can be used, copied, modified, and distributed without any fee or cost. Use of appropriate credit is requested. The software is provided as a minimum in source code form as used on USGS computers.

Center for Exposure Assessment Modeling (CEAM). CEAM was established in 1987 to meet the scientific and technical exposure assessment needs of the United States Environmental Protection Agency (U.S. EPA) as well as state environmental and resource management agencies. CEAM offers exposure assessment techniques for aquatic, terrestrial, and multimedia pathways for organic chemicals and metals.

U.S. EPA OnSite OnLine Tools for Site Assessment: Contains a suite of calculators for assessing subsurface contaminant transport.

Army Corps of Engineers. The Department of Defense, in partnership with the Department of Energy, the U.S. Environmental Protection Agency, the U.S. Nuclear Regulatory Commission and 20 academic partners, has developed the DoD Groundwater Modeling System. The

GMS provides an integrated and comprehensive computational environment for simulating subsurface flow, contaminant fate/transport, and design of remediation systems.

The Geotechnical and Geoenvironmental Software Directory (GGSD). Catalogues 1679 programs in the fields of Geotechnical Engineering, Soil Mechanics, Rock Mechanics, Engineering Geology, Foundation Engineering, Hydrogeology, Geoenvironmental Engineering, Environmental Engineering, Data Analysis and Data Visualization and lists 828 worldwide suppliers and publishers of these programs.

DEVELOP MODEL

Input Parameters

Inputs should be based on field data and, in some cases, literature values. The use of literature values may depend on how sensitive the model is to the particular parameter whether the approach is conservative, and in some cases, whether there are field methods to reliably obtain the data. Appendix A identifies common modeling input parameters and a discussion on whether site-specific or default values are appropriate. Chapter 3 (Hydrogeologic Characterization), provides additional guidance on determining site-specific values for many parameters that are needed for modeling. Inputs may need to be adjusted to calibrate the model. The modeler should demonstrate that final values lie within a reasonable range (e.g., physically realistic for the conditions).

The values of all inputs for each model node or cell should be specified in tabular or graphical form. The source of the values should be specified. Any methods used to process field-measured data to obtain model input should be specified and discussed in a report

Boundary Conditions

Types of boundaries include constant head, impermeable, constant flow, and variable head. Examples of boundaries are surface water bodies, rivers, geologic structures, injection barriers, and ground water divides. Boundary conditions are represented by mathematical expressions of a state of the physical system that refine the equations of the mathematical model. Selection of boundary conditions may have profound effects on model simulations. A model may yield biased or erroneous results if wrong boundary conditions are used.

It is desirable to represent only existing natural hydrogeologic boundaries in a model. This is possible in analytic element models and large regional numerical models that incorporate distant flow boundaries. However, many smaller site-specific numerical models employ grid systems that require an artificial boundary be specified at the edge of the grid system. In these instances, the grid boundaries should be sufficiently remote from the area of interest so that the artificial boundary does not significantly impact the predictive capabilities of the model.

Another technique for selecting appropriate boundary conditions for numerical models is to employ a stepwise or telescopic refinement modeling approach (Anderson and Woessner 1992; Feinstein et. al. 2003; Hunt et. al. 1998). In these approaches either a coarser regional numerical model or a regional analytic element model is developed, based on natural hydrogeologic boundaries, and the results from the model are used to define appropriate

boundary conditions for a smaller-scale more detailed numerical model. In some cases multiple precursor models will be developed with varying degrees of complexity, with the final result being a detailed small-scale fine-grid numerical model with boundaries based on the conditions specified from the coarser precursor models. Detailed small-scale numerical models developed using this approach will usually be more easily calibrated and provide better results than those developed with arbitrary model boundaries.

Various scenarios can be evaluated during calibration by modifying the boundaries and comparing the effects. However, once a model grid size is selected for most numerical models, it is not possible to expand the grid without creating a new model. If a numerical model was developed and there is concern that the artificial boundaries are impacting the predictive capabilities of the model, a larger scale but more simplistic analytic element model can be developed to test the influence of various boundary conditions. This approach may be simpler than developing a larger numerical model. For further information on boundary conditions, see Franke et al. (1987), Franke and Reilly (1987) and Anderson and Woessner (1992), and ASTM D5609-94(2002). A more simplistic analytic element model can also be developed to test the influence of boundary conditions on the area of interest prior to developing a more complex numerical model.

Network/Areal Grid Design

Most numerical methods require the development of an areal grid overlay. The input parameters and grid form the database on which the ground water system is defined. The formation and input of this database is specific to the computer code chosen. Fine, closely spaced grid patterns produce more accurate results. On the other hand, the finer the grid pattern, the longer the computer run time. With more recent advances in personal computers, however, computational time has become less of an issue. If computational time is not a factor and regional data is available, having a larger model area with boundaries based on actual hydrologic boundaries will be more appropriate than assigning artificial boundaries Faust and Mercer (1980) and U.S. EPA (1996a & b) provided the following general guidelines:

- Locate "well" nodes near pumping wells or near the center of a well field.

- Locate boundaries accurately. For distant boundaries, the grid may be expanded, but large spacing next to smaller ones should be avoided.

- Grid spacing should be an appropriate scale for the problem. Grid spacing should be closer together in areas where there are large spatial changes in transmissivity or hydraulic head. Large changes in hydraulic head typically occur in recharge and discharge areas, and may be especially significant near pumping wells.

- Align axes of the grid with the major directions of anisotropy (i.e., orient grid with major trends).

- Strong vertical gradients within a single saturated zone should be accommodated by multiple planes or layers or nodules.

In addition, when expanding finite difference grids beyond the interior nodes (area of modeling interest) to the boundaries, as a rule of thumb, grid spacing should not be more than 1.5 times the previous nodal spacing (Anderson and Woessner, 1992). It may be helpful to develop an analytic element model first, determine appropriate boundary conditions, and then develop a numerical model based on the information gained from the analytic element model.

Calibration

Calibration consists of changing values of input parameters in an attempt to match field conditions within acceptable criteria. Calibration requires that field conditions be properly characterized. Lack of proper characterization may result in a calibration to a set of conditions that do not represent actual field conditions. Calibration comparisons may include, but are not limited to:

- Ground water flow direction.
- Hydraulic heads and/or gradient.
- Water balance.
- Infiltration rates.
- Soil moisture content.
- Contaminant migration rates and direction (if appropriate).
- Contaminant concentrations (if appropriate).

Since some inputs (e.g., hydraulic conductivity, transmissivity, dispersivity, etc.) are highly variable, sometimes suspect, and the data is limited, these values are typically adjusted and extrapolated through an iterative process until an acceptable "match" is made. As calibration proceeds, data gaps often become evident. The modeler may have to redefine the conceptual model and collect more data. When the best calibrated match is achieved, a final input data set should be established and demonstrated to be reasonable and realistic. The degree of accuracy and how precise the match should be is governed by the defined purpose of the modeling. Each modeler and reviewer will need to use professional judgment in evaluating the results. There are no universally accepted "goodness-of-fit" criteria that apply in all cases. However, it is important that the modeler make every attempt to minimize the difference between model-simulated and field conditions. Additional information for calibrating a ground water model can be found in ASTM D5981-96(2002).

Documenting the degree of model calibration is important since it helps demonstrate how well the model estimates reality. Documentation can be in two forms: qualitative and quantitative. Qualitative is the simpler of the two, and involves using words, maps, tables and graphs to demonstrate that the model-derived predictions are consistent with the behavior that is expected based on field data. Quantitative analysis involves a statistical comparison of modeled results to values measured in the field. Many model post-processors include statistical packages that can provide an efficient tool for quantifying a model's degree of accuracy (Randazzo, 2005, ASTM D5981-02).

For initial assessments, it is possible to obtain useful results from models that are not calibrated. Potential applications include screening and guiding data collection activities.

Field-Verified

The model should be field-verified, if possible, to ensure that favorable comparisons exist between the modeled results and observed field data for the area being modeled Field verification is the process in which the calibrated model is shown to be capable of reproducing a set of field observations independent of that used in the model calibration (e.g., historical matching). The degree of verification necessary is dependent on the purpose of the modeling, type of model, results of the sensitivity analysis, and the site complexity. [Note: If the model cannot be adequately field-verified, then more emphasis should be placed on the sensitivity and uncertainty analyses.]

Sensitivity Analysis

A sensitivity analysis is the process of varying inputs over a reasonable range (range of uncertainty in the value of the parameter) and observing the relative change in model response. The sensitivity of one parameter versus others is also evaluated. Typically, the observed changes in hydraulic head, flow rate, or contaminant transport are noted. The purpose of the sensitivity analysis is to demonstrate the sensitivity of the simulations by varying input values. If some change in a parameter or boundary condition causes significant changes in output, then the model is sensitive to that parameter or boundary. For example, the modeled hydraulic conductivity is varied between 100 and 500 feet/day and the heads in the model do not vary significantly, it could be interpreted that the particular model is not sensitive to K. However, if riverbed conductance is varied from 1 to 100 days and the modeled heads vary significantly, then the model could be interpreted to be sensitive to river conductance.

Sensitivity analyses are also beneficial in determining the direction of future data collection activities. Data for which a model is relatively sensitive would require future characterization, as opposed to data for which the model is relatively insensitive, which would not require further field characterization. For additional information, see Anderson and Woessner (1992); Zheng and Bennett (1995), and ASTM D5611-94(2002).

Uncertainty Analysis

An uncertainty analysis is conducted by assigning distributions to parameters that are demonstrated to have the most variability in the field and are demonstrated to be the most sensitive to the model output. Various methods for introducing uncertainty into the models and the modeling process have been proposed. For example, one approach is to employ Monte Carlo methods in which the various possibilities are represented in a large number of simulated realizations. Another approach is to construct stochastic models in which the various coefficients are represented as probability distributions rather than deterministic values (Bear et al., 1992).

PREDICTION

Upon completing calibration, sensitivity analysis, and field-verification, the model can be used to predict future scenarios. Such simulations may be used to estimate the hydraulic response of a zone, the possible migration pathway of a contaminant, the contaminant mass removal rate, or concentrations of a contaminant at a point of compliance at some future point in time.

Predictive simulations can also be used to predict responses to the system as natural- or man-induced stresses are applied. For example, a model may be used to predict the pumping rate needed to capture a contaminant plume and to estimate the contaminant concentration of the extracted ground water. Monitoring of hydraulic heads and contamination concentrations should be used to verify hydraulic containment and remediation.

The predictive simulations should be viewed as estimates and not as a certainty. There is always some uncertainty in predictive models. The simulations are based on the conceptual model, the hydrogeological and geochemical input parameters, and the model algorithms. The model's limitations and assumptions, as well as the differences between field conditions and the conceptual model will result in errors in simulations. In an attempt to minimize these errors, models are calibrated by adjusting inputs until the model closely reproduces field conditions within some acceptable criteria. However, the time period over which a model is calibrated is typically small compared to the length of time used for predictive simulations. Relatively small errors observed during the time period over the model calibration or history matching may be greatly magnified during predictive simulations because of the larger time period typically used in predictive simulations. The growth in errors resulting from projecting model simulation into the future may need to be evaluated by monitoring field conditions over the time period of the simulation or until appropriate cleanup criteria have been achieved.

Predictive simulations are often conservative. That is, given the uncertainty in model input parameters and the corresponding uncertainty, model input values are selected that result in a "worst-case" simulation. Site-specific data may be used to support a more reasonable worst-case scenario. Or stated another way, site-specific data should be collected to limit the range of uncertainty in predictive models. If long-term action is necessary, it may be necessary to refine and update the model as additional data are collected and future stresses are observed (see Performance Monitoring section).

PERFORMANCE MONITORING ("Validation")

A sufficiently calibrated and field-validated model uses historical data to predict the future; however, it is difficult to predict the magnitude, location, and duration of future stresses. As a result, performance monitoring (validation) of predictive simulations often show the flow system did not behave as predicted. Post-audits utilize the additional field data collected after the model study is completed to evaluate the accuracy of the prediction. The new data should be used to recalibrate the model to update and improve the simulation. These periodic updates allow appropriate "corrective actions" to be made (e.g., modifications to an extraction well system). Anderson and Woessner (1992) and Konikow (1986) provided discussions on post-audit methods that can be utilized to re-calibrate a model. Many investigators have suggested not extending transient predictive simulations for more than twice the number of years for which there is transient calibration and verification data (Faust et al., 1981).

DOCUMENTATION OF MODEL RESULTS

Documentation of a model is important to show that the interpretations made reasonably represent site conclusions. This will facilitate peer review and also enable further scientific verification by allowing the model to be reproduced by future modelers. Results should be

presented clearly and concisely and include appropriate documentation. Model documentation includes written and graphical presentation of the assumptions and objectives, the conceptual model, code description, model construction, calibration, predictive simulations, and conclusions. The following provides an outline of components that should be incorporated into a report (ASTM D5718-95 (2006), Anderson and Woessner (1992), Mandle (2002)):

- ***Purpose*** - The purpose and specific goals or objectives of the modeling should be clearly stated. It should be documented that the objectives of the simulation correspond to the decision-making needs.

- ***Hydrogeologic Setting*** - A narrative, with appropriate cross-sections and maps of the hydrogeologic system, should be provided. The data used (e.g., borings, well logs) should be provided or referenced to where the data can be obtained.

- ***Data Collection*** - Methods and techniques for collecting, analyzing and interpreting data should be explained. Levels of confidence for system parameters should be discussed. Any data gaps and simplifying assumptions should be discussed. Data set strengths and deficiencies should be noted.

- ***Detailed Conceptual Model*** - It should be documented that the conceptual model is consistent with the site's physical and chemical processes. Any uncertainties and simplifying assumptions should be justified.

- ***Model Description*** - The rationale for the choice of a particular model should be documented. Simplifying assumptions and limitations of the model should be discussed and related to the problem to be simulated, along with the impact these assumptions may have on the results. A description of where assumptions and actual field conditions do not coincide should be presented. It should be shown that the model chosen is appropriate for the system. Any modifications to the code should also be discussed.

- ***Model Construction -*** The layering and gridding of the model should be described. This would include describing how pumping wells and natural boundary conditions are represented. Document whether the grid selection was appropriate for the scale of the problem.

- ***Assignment of Model Parameters*** - It should be shown that there are sufficient data to characterize the site and satisfy the data needs of the model. All input data, including initial conditions, boundary conditions, and hydraulic and transport parameters, should be defined. The reasons for selecting initial and boundary conditions should be justified. Assigned values throughout the modeled area should be presented. Data can be presented on cross-sections and maps showing flow boundaries, topography and surface water features, water-table/potentiometric surfaces, bedrock configuration, saturated thickness, transmissivity/hydraulic conductivity, specific storage, cross sections, etc. All sources of data used, whether derived from published sources, measured, or calculated from field data or laboratory testing should be documented.

- ***Model Calibration*** - Specific goals and procedures of calibration, results of the final calibrated model, departure from the calibration targets, the effects of the departure on the model results, and the overall water and/or chemical balance of the model should be presented and discussed.

- ***Sensitivity Analysis*** - All sensitivity analyses should be presented and interpreted. Input parameters that have the greatest impact on results should be described.

- ***Field Verification***- Goals and procedures of any field verification should be presented and discussed. Additional sensitivity analyses on these new comparisons should be documented.

- ***Data Pre- and Post-Processing*** - All pre- and post-processing of model input and output data should be described and any computer codes utilized should be documented. The modeler(s) should describe the data manipulation process and why it was conducted.

- ***Model Prediction-*** All output from predictive simulations should be presented and interpreted in detail. The modeler(s) should cover model water balance, highlighting salient features such as pumpage, recharge, leakage, etc. All predictions should be presented in the context of the fundamental assumptions of the model. Limitations of and confidence in predictions should also be stated.

- ***Sources of Error-*** Known problems and errors may need to be evaluated and discussed by utilizing ranges and expressing levels of confidence for predictions made. Konikow (1988) identified several common types of predictive errors. Sources of error are also discussed in ASTM D5880-95(2006).
- ***Summary and Conclusion*** – Summarize the modeling effort and draw conclusions related to the study objectives. The limitations of the modeling and all assumptions should be discussed. Also, discuss uncertainties inherent to the model and their effects on conclusions.

- ***Model Records*** - The entity should keep on file, and be able to provide upon request, input and output data sets for model runs (in digital form or hard copy), including final calibration, additional history matching, and all predictions. The original model documentation and a copy of the source code used should also be available upon request.

- ***Post Audit*** - If a model will be used to make decisions that extend beyond its predictive limit, the report should include a plan for future ~~post-audits~~ evaluations to check the model in time and space to be certain that past decisions are still appropriate.

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APPENDIX A
COMMON MODELING INPUTS

HYDROGEOLOGIC INPUTS

Hydraulic Conductivity

Hydraulic conductivity **(**K) is a coefficient of proportionality describing the ease at which fluid can move through a permeable medium and is expressed in units of length per time. It is a function of properties of both the porous medium and the fluid. In most cases, site-specific values should be used for both vertical and horizontal K. It is generally a sensitive modeling input parameter. Methods to determine K are described in Chapter 3.

If an insufficient amount of site-specific data exists or the site is more complex than the model can handle, then literature values are often used to support the model. However, models relying on literature data would need to rely on good sensitivity and uncertainty analysis.

Intrinsic Permeability

Site-specific hydraulic conductivity is generally determined in a site investigation. However, some models use intrinsic permeability instead of hydraulic conductivity. Intrinsic permeability describes the ease with which a porous medium can transmit a liquid under a hydraulic or potential gradient. It differs from hydraulic conductivity in that it is a property of the porous media only and is independent of the nature of the liquid. For water, it is related to hydraulic conductivity by

$$k = \frac{K \times \mu}{\rho \times g} = 10^{-5} \mathrm{m} \cdot \mathrm{s}$$

k = intrinsic permeability cm^2
K = hydraulic conductivity cm/sec
μ= dynamic viscosity g/cm-sec (0.01 g/cm sec)
ρ = density of fluid g/cm^3 (0.99821 g/cm^3)
g = acceleration of gravity cm/sec (980 cm/sec^2)

Hydraulic Gradient

Hydraulic gradient is the total change in head with change in distance in the direction of flow. The gradient generally is analogous to the slope of the potentiometric or water table surface. It is generally a sensitive input. Hydraulic gradient is generally entered as a value in analytical model, while hydraulic heads are generally input into numerical models. Methods to determine hydraulic gradient can be found in Chapter 3.

Bulk Density

Bulk density (also called dry bulk density) is the ratio of the mass of dry solids to the bulk volume of a soil. The bulk density is therefore less than the density of particles that make up the soil, because it also includes the volume of pore space. It is used by geotechnical engineers to estimate compaction of the soils. Bulk density is used in modeling to calculate

between the volumetric water content and the gravimetric water content, to calculate retardation factors, and is coupled with the particle density to calculate the porosity of a soil.

There is no standard method for measuring of bulk density. Most commonly, dry bulk density is measured by taking a sample of known volume, drying it at 105°C for 24 hours or until a constant weight is obtained, then weighing the dried soil sample. The dry weight divided by the volume is the bulk density (Ohio EPA, 2003b). Other methods to measure bulk density include radiation techniques (Blake and Hartge,1986). Site-specific bulk density also can be determined by ASTM D2167-94 (2001), D2922-05, and D2937-04.

The dry bulk density will vary within certain limits for different soil types. Range of default values for various media can be found in Table A14.1. In most cases, bulk density is not a sensitive parameter and these values may be used as defaults in models. A sensitivity analysis should be provided unless the model documentation indicates the bulk density is not sensitive.

Table A14.1 Bulk Density (Jury,1986).

Soil Type	Bulk Density (g/cm3)
Sand	1.59 - 1.65
Sandy Loam	1.2 - 1.49
Silt loam	1.47
Clay Loam	1.2-1.36
Silty clay	1.26

Porosity/Effective Porosity

Porosity is the ratio of openings to the total volume of rock and soil. The pore space and the arrangement of pore spaces within a soil sample are very complex and difficult to measure. This is because the arrangement of soil particles influences the shape, size and orientation of pores within the soil matrix. The porosity of a soil will vary with the arrangement of particles or texture. In general, finer grained soils, rich in clay, will have the highest porosity, and coarser textured soils, rich in sand, will have lower porosity.

Porosity (n) can be calculated by a variety of means. The most common is to calculate the percentage of total soil volume occupied by pores. This is done by calculating a soil's bulk and particle density (Blake and Heritage, 1986) and using:

$$\text{porosity } (n)=[1-\frac{\text{bulk density}}{\text{particle density}})]$$

Typical porosities are listed in Table 14.2 and in TGM Chapter 3, Table 3.9. On average, particle densities of 2.65 g/cm3 are typical of sandy soils but decrease as the clay and organic matter content rise.

Another method is to use pycnometry as described by Danielson and Sutherland (1983). Porosity measurements are important and are used in most ground water and fate and

transport models. These measurements serve as a basis for determining the water-filled porosity, air-filled porosity and in calculations to determine the total mass of contaminants.

Not all of the porosity is available for flow. Part will be occupied by static fluids being held to the soil/rock by surface tension or contained in dead end pore spaces. The porosity available for fluid flow is the effective porosity. It is also a function of the size of the molecules that are being transported to the relative size of the passageways that connect the pores. Therefore, the effective porosity for solute transport may differ from that of water for the same material.

Effective porosity is difficult to measure and is typically selected by experience and intuition. Effective porosity is generally estimated based on the description and classification of subsurface materials and by total porosity, determined from lab tests or estimated from the literature. Tables A14.2 and A14.3 provide data that might be useful to this estimation. Peyton et al. (1986) found that even in lacustrine clay, water molecules could pass through all pore throats, so that effective porosity was essentially the same as porosity (Fetter, 2001). This suggests that, for at least water, effective porosity may be considered equal to total porosity.

For unfractured glacial till, it is recommended that 30 percent be used for n_e in velocity calculations[7]. While a default value of one percent has been cited for clay (U.S. EPA, 1986), this results in high rates that are intuitively incorrect. Primary flow through clay is known to be very low. This 30% compares favorably with the value for clays reported by Rawls et al. (1983) (Table A14.2). Ohio EPA's experience is that use of 30 percent results in very conservative estimates of ground water movement through unfractured glacial till.

[7]It should be noted that the applicability of Darcy's law to calculating primary flow velocity in fine-grained material is questionable. However, this currently is one of the best available tools to assist professionals in evaluating whether a confining unit provides protection to the underlying ground water. To further demonstrate that ground water has not/will not be affected by a potential contaminant source, other methods such as tracers may be helpful.

Table A14.2 Porosity and Effective Porosity of Common Soils (Rawls et al., 1983).

Texture	Mean Total Porosity	Mean Effective Porosity
Sand	0.437	0.417
Loamy Sand	0.437	0.401
Sandy Loam	0.453	0.412
Loam	0.463	0.434
Silt Loam	0.501	0.486
Sandy Clay Loam	0.398	0.330
Clay Loam	0.464	0.309
Silty Clay Loam	0.471	0.432
Sandy Clay	0.430	0.321
Silty Clay	0.479	0.423
Clay	0.475	0.385

Table A14.3 Range of percentage of porosity for various geologic materials.

GEOLOGIC MATERIALS	BOUWER (1978)	TODD AND Mays (2004)	FETTER (2001)	FREEZE AND CHERRY (1979)	SEVEE (2006)
gravel, mixed	20-30			25-40	25-40
gravel, coarse		28			
gravel, medium		32			
gravel, fine		34			
sand, mixed	25-50			25-50	15-48
sand, coarse	25-35	39			
sand, medium	35-40	39			
sand, fine	40-50	42			
sand & gravel	10-30		25-50		
silt	50-60	46	35-50	35-50	35-50
clay	50-60	42	33-60	40-70	40-70
glacial till	25-40	31-34	10-20		
limestone	10-20	30		0-20	0-20
shale		6		0-10	0-10
sandstone	5-30	33-37		5-30	5-40

Water Content

Water content indicates the amount of water in a soil sample. In the vadose zone, this value will change over time as the soil water budget changes. Most vadose zone models require some measure of water content. However, there is some confusion about the basis for water content measurement and the use of the data. The most common measurement is the percent moisture content of a soil sample. The measurement is made by weighing a soil sample, drying it at 105 ℃ until a constant weight is obtained, then weighing the dried soil sample. The percent moisture content is then:

$$\%\,\text{moisture} = \frac{\text{wet weight -dry weight}}{\text{dry weight}} \times 100 \qquad (1)$$

The ratio of dry weight to wet weight of a soil sample represents the gravimetric water content or water content on a mass basis (θ_m). Unfortunately, most vadose zone models require that water content of a soil be expressed in terms of volumetric water content (θ_V). The conversion from water content based upon mass to that of a volumetric basis can be made with the following relationships:

$$\frac{\text{volume of water (ml)}}{\text{volume of soil (ml)}} = \theta_m \left(\frac{g}{g}\right) \times \frac{\text{bulk density } \left(g/cm^3\right)}{\text{density of water } \left(g/cm^3\right)} \qquad (2)$$

where the bulk density is defined previously and density of water is usually assumed to be 1.0 g/cm3.

In many applications, the model prompts the user for neither the volumetric nor mass water content. Instead, it requires water-filled porosity or the percentage that the average pore-space is filled with water. This value can be determined by first noting that:

$$\text{volume of pore space (mL)} = \text{porosity} \times \text{volume of Soil (mL)} \qquad (3)$$

Rearranging equation 3 in terms of volume of soil and substituting this relation in equation 2, the following relationship is found:

$$\frac{\text{volume of water (mL)}}{\text{volume of soil (mL)}} \times \frac{\theta_m \left(\frac{g}{g}\right)}{\text{porosity}} \times \frac{\text{bulk density } \left(\frac{g}{cm3}\right)}{\text{density of water } \left(\frac{g}{cm3}\right)} \qquad (4)$$

This ratio is then multiplied by 100 to determine the percentage of water in the pore space of a soil sample. For example, if a sample is determined to have 20% moisture content (determined on a mass basis), a dry bulk density of 1.5 g/cm3 , a total porosity of 0.5 (i.e. 50%) and the density of water is 1.0 g/cm3, then:

$$\% \text{ of pore filled with water} = \frac{0.2}{0.5} \times \frac{1.5(\frac{g}{cm3})}{1.0(\frac{g}{cm3})} \times 100 = 60\%$$

FATE AND TRANSPORT INPUTS

Dispersion Coefficients

Dispersion (or dispersvity) is the spreading of a solute caused by mechanical dispersion and molecular diffusion:

- Mechanical dispersion results from ground water moving at rates both greater and less than the average linear velocity. This is due to: 1) fluids moving faster through the center of the pores than along the edges, 2) fluids traveling shorter pathways and/or splitting or branching to the sides, and 3) fluids traveling faster through larger pores than through smaller pores (Fetter, 2001). Because the invading solute-containing water does not travel at the same velocity, mixing occurs along flow paths. This mixing is called mechanical dispersion and results in distribution of the solute at the advancing edge of flow (Fetter, 1993). The mixing that occurs in the direction of flow is called longitudinal dispersion. Spreading normal to the direction of flow from splitting and branching out to the sides is called transverse dispersion.

- Molecular diffusion is the process by which ionic and molecular species dissolved in the water move from areas of higher concentration (i.e., chemical activity) to areas of lower concentration. Diffusion is an important process influencing contaminant migration in unfractured clayey aquitards.

Mechanical dispersion and molecular diffusion cannot be distinguished in a ground water flow system and often are referred to collectively as hydrodynamic dispersion (Fetter, 2001). Depending on the degree of dispersion, a contaminant may form a wide or a narrow plume. Hydrodynamic dispersion phenomena also may cause contaminants to arrive at a given location significantly ahead of the arrival time expected solely from an average flow rate. General textbooks by Freeze and Cherry (1979), Fetter (2001), Luckner and Schestakow (1991), Domenico and Schwartz (1990), and Fetter (1993) should be consulted for additional information on hydrodynamic dispersion.

Many models require a dispersivity term to account for both mechanical dispersion and diffusion. Due to the impracticability of measuring dispersion in the field, dispersivity values are often estimated based on plume length or distance to receptors. Gelhar et al. (1992) cautions that dispersivity values vary between 2-3 orders of magnitude for a given scale due to natural variation in hydraulic conductivity. Therefore dispersivity values can be manipulated within a large range and still be within the range of values observed at field test sites.

Longitudinal dispersivity (a_L), which is a measure of the “spread” of the plume in the direction of flow, can be estimated based on a formula developed by using a weighted best fit of field data (Xu and Eckstein,1995). This equation is provided below and can also be found on

U.S. EPA On-Line Tools for assessing longitudinal dispersivity. (Note: Equation is specific to units (e.g., metric)).

$\alpha_L = 0.83 \times (\log L_p)^{2.312}$ α_L = Longitudinal dispersivity (m)
L_p = Plume length (m)

Other commonly used relationships for dispersivity include:

$\alpha_L = 0.1 L_p$ (U.S. EPA 1996)

$\alpha_v = 0.0056 L_p$ (Gelhar and Axness, 1981)

$\alpha_T = 0.10\ a_L$ (Gelhar and Axness, 1981)

Where: α_L = Longitudinal dispersivity (m)
α_v = vertical dispersivity (m)
α_T = transverse dispersivity (m)
L_p = Plume length (m)

Fraction of Organic Carbon

The fraction of organic carbon (f_{oc}) is the carbon in the soil that is made up of decaying plant and animal matter, humus, *etc.* It is differentiated from inorganic carbon (typically in calcium or magnesium carbonates), which does not have the same effect on contaminant movement. The fraction of organic carbon is generally the dominant retarding mechanism for contaminant movement in the vadose zone.

Organic carbon and matter contents of soils can have a significant effect on fate and transport; therefore, accurate determination is important and sampling and analysis should be performed with great care. For site-specific modeling, the practitioner should collect a representative number of samples, both horizontally and vertically, over the affected area. Analytical methods to determine organic matter can be found in ASTM D2974-00 or Soil Science Society of America Methods (Nelson and Sommers, 1996). Commonly, modified ground water methods for total organic carbon are used by commercial laboratories and, in general, these methods can overestimate the amount organic carbon in soils. This is because inorganic carbon is not distinguished by the analytical method. The practitioner is directed to the methods of analysis outlined by Nelson and Sommers (1996), which will give an accurate account of soil organic carbon content. Methods such as SW-846 Method 9060A (U.S.EPA, 2004) should not be used to determine the organic carbon content of soils without modification. Additional information can found in VAP TDC document VA30007.03.019 (Ohio EPA,2003a).

If site-specific values are not determined, acceptable defaults for sand, silt, and clay are 0.2, 0.25 and 0.3, respectively.

Partitioning

Partitioning is a process in which chemicals are distributed between solid, liquid, and gas phases, depending upon solubility, sorption, and vapor pressure characteristics.

Soil Organic Carbon-Water Partitioning Coefficient

The soil organic carbon-water partitioning coefficient (K_{OC}) is the ratio of the mass of a chemical that is adsorbed in the soil per unit mass of organic carbon in the soil per the equilibrium chemical concentration in solution. K_{OC} values are useful in predicting the mobility of organic soil contaminants; higher K_{OC} values correlate to less mobility chemicals, while lower K_{OC} values correlate to more mobility. K_{oc} values can vary greatly in the literature, and a sensitivity analysis may be needed. However, depending on the regulated program, Ohio EPA will generally accept the values listed in Table 3 of the Division of Hazardous Waste Management, Closure Review Guidance (2006), or the Division of Emergency and Remedial Response, Voluntary Action Program, Support Document for Development of Generic Numeric Standards and Risk Assessment (Ohio EPA, 2002).

The coefficients presented in these papers are not applicable for situations where mobilization is from enhanced solvation. The Kd values presented assume that relatively dilute solution conditions are present, that a narrow range of soil moisture content is applicable and that a consistent range of soil organic matter is present. If these basic assumptions are not met, site-specific determination of the leaching of inorganic substances is warranted.

Distribution Coefficient

Distribution coefficient (Kd) is the ratio of a chemical's sorbed concentration (mg/kg) to the dissolved concentration (mg/L) at equilibrium. For organics, Kd may be calculated by multiplying Koc (the soil organic carbon-water partitioning coefficient) by the fraction of organic carbon (foc):

$$Kd = Koc \times foc$$

For metals, acceptable values for several metals can be found in Table 3 of Ohio EPA's, Division of Hazardous Waste Management, Vadose Zone Modeling for RCRA Closure (Ohio EPA, 2003b).

Relative Solubility

Relative solubility controls whether a contaminant exists in ground water primarily as a dissolved (soluble) or free liquid phase (insoluble). Movement of the dissolved phase is generally in the direction of flow and is governed primarily by the processes of advection-dispersion and biological/chemical attenuation. Literature values are generally acceptable for solubility and the values provided in guidance listed under the Koc section are acceptable.

Henry's Law Constant

At a constant temperature, the amount of a given gas dissolved in a given type and volume of liquid is directly proportional to the partial pressure of that gas in equilibrium with that liquid. Note that care should be taken to determine the units of Henry's Law constant. Some models require the term to be in m^3-atm/mol while other models require it to be dimensionless.

Variation of Henry's Law constant can affect model results. The high Henry's Law constant of some volatile organics controls volatilization in the subsurface, dominating other pollutant loss mechanisms. Hence, a slight change may affect the model. However, Henry's Law constants do not vary to a great degree as reported in literature. For ground water and subsurface fate and transport models, acceptable default values are listed in Table 3 of the Division of Hazardous Waste Closure Review Guidance (Ohio EPA, 2006), or the Division of Emergency and Remedial Response, Voluntary Action Program, Support Document for Development of Generic Numeric Standards and Risk Assessment (Ohio EPA, 2002).

Degradation

Degradation of contaminants in the environment can be biotic (biologically mediated) or abiotic (chemical reaction). It accounts for the loss of a pollutant and the formation of daughter products. If the degradation process is accounted for, but not properly justified, predicted concentrations of a pollutant could be underestimated. Likewise, if degradation is occurring, but not accounted for, daughter products, which may be more toxic than the parent compound, may not be properly addressed.

Many models incorporate degradation as a first order decay rate. The user is responsible for demonstrating whether degradation is occurring, what degradation products will form, and the significance of the degradation products

Literature values for biodegradation rates are highly variable and are often based on laboratory testing or in field conditions where the factors affecting biodegradation can be controlled. The *Committee on In Situ Bioremediation*[1] recommends that the effectiveness of intrinsic bioremediation should be continually monitored by analyzing the fate of the contaminants and other reactants and products indicative of bioremediation. This monitoring includes three types of information: documented loss of contaminants from a site, laboratory assays showing that the microorganisms from site samples have the potential to transform contaminants under the expected site conditions, and confirming evidence that the biodegradation potential is actually realized in the field. Additional information on biodegradation can be found in ASTM E1943-98 (2004), US EPA, (1998), ITRC (1999), and

1 The Committee on In Situ Bioremediation was established in 1992 with the specific task of developing guidelines for evaluating in situ bioremediation projects and determining whether they are or will meet clean-up goals. It represents the span of groups involved in bioremediation: buyers of bioremediation services, bioremediation contractors, environmental regulators, and academic researchers.

NRC (2000). The user should consult with the regulatory program to determine whether literature values of degradation are acceptable and if so, how they can be applied.[1]

Source Size

Sufficient data needs to be collected to adequately determine or estimate the source or plume size both vertically and spatially.

Initial (concentration) Inputs

Initializing the plume concentration needs to be assessed. Whether to use the maximum or average may be dependent on the purpose of the model, amount of data, and the complexity of the chosen model. It is recommended that the user consult with the regulatory program to develop an acceptable approach.

[1] For RCRA Closures, the Division of Hazardous Waste Management will not accept literature values for biodegradation of organic chemicals. If biodegradation rates are included in a model, site-specific data, including the methods used, number of samples, and laboratory data reports must be supplied to verify these inputs. For DERR/VAP properties see TDC document VA 30007.97.004 (Ohio EPA, 1997).

APPENDIX A
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