GEORGIA
DEPARTMENT OF NATURAL RESOURCES
ENVIRONMENTAL PROTECTION DIVISION

Land Protection Branch

Guidance:
Groundwater Contaminant Fate and Transport Modeling

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1.0 INTRODUCTION

The purpose of this guidance is to provide general guidelines for the application of groundwater contaminant fate and transport models, including the planning and evaluation of models for use at sites with groundwater contamination that are subject to regulation by the Georgia Environmental Protection Division (EPD) under the following statutes:

- Federal Resource Conservation and Recovery Act (RCRA)
- Federal Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)
- Georgia Hazardous Waste Management Act, O.C.G.A. 12-8-60
- Georgia Hazardous Site Response Act (HSRA), O.C.G.A. 12-8-90
- Georgia Voluntary Remediation Program Act (VRPA), O.C.G.A. 12-8-100
- Georgia Brownfield Act, O.C.G.A. 12-8-200
- Georgia Underground Storage Tank Act, O.C.G.A. 12-13-1
- Georgia Solid Waste Management Act., O.C.G.A. 12-8-20

Regulatory oversight of the above statutes is administered by the following programs within the EPD Land Protection Branch:

- Response and Remediation Program (including the Brownfields Unit)
- Solid Waste Management Program
- Underground Storage Tank Management Program
- Hazardous Waste Management Program
- Hazardous Waste Corrective Action Program

This guidance outlines recommended practices and explains their rationale. However, EPD may not require an entity to follow methods recommended by this or any other guidance document. The entity may however need to demonstrate that an alternate method produces data and information that meet the pertinent requirements. This guidance *is not a substitute for professional judgment*, which must be applied in the selection and application of fate and transport modeling, *nor does it advocate modeling over the collection and interpretation of quality media-specific site data*.

This document describes the process of preparing a fate and transport model for consideration. Each section provides a brief discussion of each step and the rationale for its use. Figure 1-1 outlines the steps that are typically involved in groundwater contaminant fate and transport model application at contaminated sites. Additional steps may be necessary to meet modeling objectives. For example, a site investigation may provide additional data that can be used in the modeling process. The development of a Modeling Work Plan may assist EPD in determining if the proposed modeling is appropriate.

2.0 DEFINE MODELING OBJECTIVES

The objective(s) for the modeling should be specific and measurable. Acceptable objectives for groundwater contaminant fate and transport modeling will vary dependent upon the statute under which a particular site is administrated. The ultimate objective of EPD is protection of human health and the environment. Groundwater contaminant fate and transport modeling is a potential tool that can be used, along with others, to achieve that objective.

The modeling report must demonstrate that the objectives of the specific regulatory program under which the site is administrated, *and* this guidance, have been met by the model.

3.0 DATA REVIEW

Available data should be included as part of a Conceptual Site Model (CSM). Some EPD programs require a summary of the available data be submitted as part of the CSM. The CSM may also identify gaps in the data to be used in modeling. Regardless of how data are presented, the sources and validity of data used in modeling must be documented. Any manipulation (*i.e.*, exclusion, statistical analysis, *etc*.) of data used in modeling must also be thoroughly documented and justified.

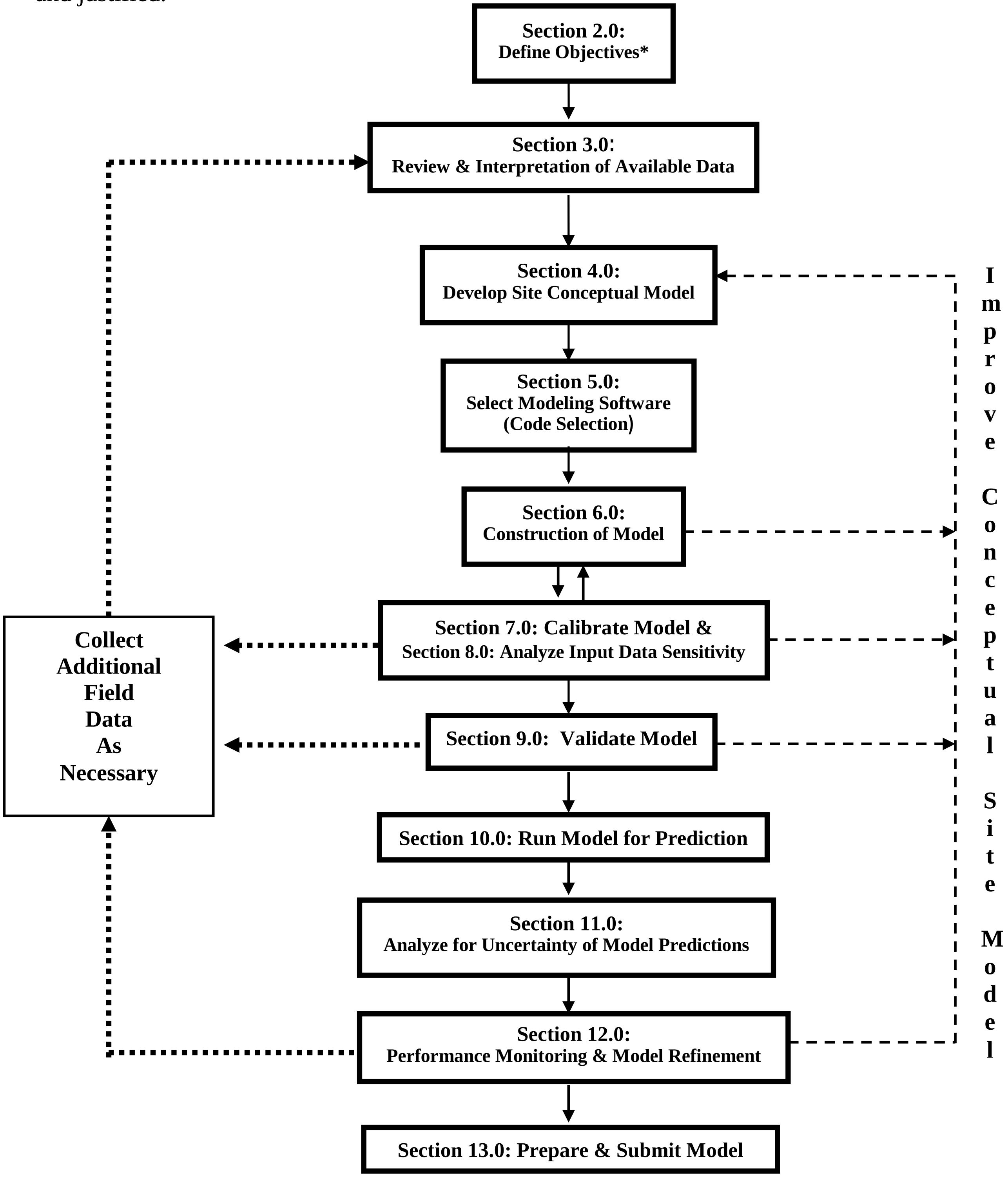

Figure 1-1: Steps in Groundwater Contaminant Fate & Transport Modeling Application
(Modified from Bear, et. al., April 1992)

***Note:** At any time in the model application process it may become apparent that objectives should be refined or redefined based on availability of data, inability to calibrate or validate the model, etc.*

4.0 CONCEPTUAL SITE MODEL

Guidance on how to develop a CSM is readily available from other state agencies, federal agencies, and private organizations such as the American Society for Testing and Materials (ASTM; ASTM E1689-95), and will not be covered in detail here. The purpose in developing a CSM is to document physical and chemical site conditions that affect contaminant fate and transport. Developing a CSM may allow EPD to verify that the modeling adequately represents site conditions. In some cases, the CSM required by the Voluntary Remediation Program may be adequate for modeling.

The CSM should be as simple as possible, while retaining sufficient complexity to adequately represent the physical and chemical elements of the system. For instance, a site with a single homogeneous, isotropic, water-bearing unit with one direction of groundwater movement and a single constituent of concern may only require a simple CSM. A site with multiple water-bearing units, more than one direction of groundwater movement and multiple constituents of concern may require a more complex CSM.

A CSM may address, but not necessarily be limited to, site conditions such as:

- One-dimensional or multi-dimensional contaminant transport
- Steady-state or transient conditions
- Unconfined or confined aquifers
- Homogeneous/isotropic or heterogeneous/anisotropic aquifers
- Dip/Attitude of water-bearing unit(s)
- Constant or variable groundwater velocity, hydraulic head, *etc*.
- Variable or constant/uniform, groundwater flow direction/paths
- Contaminant concentrations, dispersion, adsorption/retardation and biodegradation/ transformation
- Continuous or instantaneous/finite source
- Variable source concentrations
- Mass transport
- Mixing of water-bearing units
- Chemical specific properties, *etc.*

A CSM should be updated if and as more site-specific data become available, *or* if site conditions change. Some EPD programs [*e.g*., the Voluntary Remediation Program (VRP)] require the CSM to be periodically updated and reported.

5.0 COMPUTER MODEL SOFTWARE SELECTION

A list of software available for contaminant fate and transport modeling is not included in this guidance. The nature of transport media, contaminant type and distribution, modeling objectives, and the complexity of site conditions require that models should be evaluated on a site-specific basis. Lists of fate and transport models, and supporting guidance, are available from many sources, including:

- U.S. EPA's Center for Subsurface Modeling Support (CSMoS)
- U.S. EPA's Center for Exposure Assessment Modeling in Athens, Georgia
- U.S. Geological Survey (USGS)
- Air Force Center for Environmental Excellence (AFCEE)
- International Groundwater Modeling Center (IGWMC)

The model used may be analytical, numerical, or any combination thereof and should include user documentation that a reviewer could use to set up and run the model and understand model outputs. Georgia EPD will consider models using software developed by the U.S. Environmental

Protection Agency, the U.S. Geological Survey, and the U.S. Departments of Defense or Energy. EPD may consider models developed using other software, if documentation is provided to EPD demonstrating the software has been verified, peer-reviewed and well documented. If the software is required to review the model and the software cannot be obtained without cost, a copy of the software and a license to view the software must be provided to EPD. Any analytical model must meet regulatory and program-specific requirements.

6.0 CONSTRUCTION OF THE MODEL

Inputs should be based on field data and, in some cases, appropriate peer-reviewed literature values. The use of literature values may depend on how sensitive the model is to the particular parameter, whether the approach is conservative (*i.e.,* will result in over-estimated rather than under-estimated contaminant concentrations and contaminant migration), and in some cases, whether there are field methods to reliably obtain the data. 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, graphical, or map format. 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 the report.

The design of the groundwater model should adequately represent the data available for modeling and the conceptual site model, and meet the modeling objectives. Where applicable, the model design should include, but not be limited to:

- Model layering and grids
- Aquifer and confining unit hydraulic properties
- Boundary conditions
- Aquifer recharge and discharge
- Interactions between groundwater and surface water
- Groundwater flow and chemical interactions with the aquifer(s) that cause retardation of constituent movement
- Baseline Stresses such as existing groundwater pumping from wells
- The ability of the model to run steady state or transient simulations or both
- Other pertinent features of the model

Basic aspects of hydrogeology that should be considered in constructing a model are presented in Appendix A of this Guidance.

6.1 Model Layering

Some models consist of a single layer and some consists of multiple layers to represent an aquifer system. Model layers and identification of confined and unconfined aquifers should be consistent with the site hydrogeology represented in the CSM. If the aquifer system consists of multiple layers, and the software can only model a single layer, multiple models may need to be run for each layer in the aquifer system. If a CSM indicates that there are multiple layers within the aquifer system through which contaminant transport may occur, it may be better to use alternate software capable of modeling multiple layers. Grids (where used) should be spaced adequately to provide the required level of model output detail, appropriate aspect ratios, and aligned consistent with boundary conditions.

6.2 Aquifer and Confining Unit Hydraulic Properties

Hydraulic properties are the aquifer properties that regulate the transmission and storage of water and movement of constituents in those media such as:

- Horizontal Hydraulic Conductivity (K_h)
- Vertical Hydraulic Conductivity (K_v)
- Transmissivity (T)
- Total Porosity (n_t)
- Effective Porosity (n_e)
- Saturated Thickness of Aquifer (b)
- Seepage Velocity (V_{sx})
- Darcy Velocity (V_x)
- Specific Yield (S_y)
- Storativity/Storage Coefficient (S)
- Specific Storage
- Streambed Conductance
- Leakance
- Bulk Density (ρ_b)
- pH
- Fraction of Oganic Carbon (f_{oc})

Some models may include other hydraulic properties that are not listed above. Hydraulic properties used in the model should be consistent with peer-reviewed publications or field measured values, or both.

Key input parameters for modeling fate and transport of organic and inorganic contaminants are f_{oc} and pH, respectively. Contaminant fate and transport models are often very sensitive to these parameters. Therefore, values of these parameters must be justified and conservative.

6.3 Boundary Conditions

Types of boundaries that should be evaluated include constant head, impermeable, constant flow, variable head, and mixed. Examples of boundaries include: 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. Boundaries of the modeled domain should preferably be, or correlate with, existing physical boundaries. Groundwater divides may at times be chosen as domain boundaries, but they are not fixed physical boundaries in that they can change location or disappear as a result of different stresses upon the hydrologic system. Accordingly, the use of a groundwater divide as a model boundary may produce inconsistent or errant results. It is appropriate that only existing natural hydrogeologic boundaries be represented in a model. This is possible in analytical 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. When using artificial boundaries, the effects of boundary conditions on a particular area can be tested by adjusting the boundary conditions to determine the effects on model results.

6.4 Aquifer Recharge and Discharge

Where applicable, aquifer recharge and discharge rates and volumes should be consistent with the CSM and how interactions between groundwater and surface water were modeled. Recharge can be simulated using specified head or flow boundaries, or by specifying recharge to be a surficial layer of a numerical model. Not all modeling programs will allow for input of recharge.

6.5 Chemical Properties and Transport Processes

Physical- and chemical-property values may include, but not necessarily be limited to:

- Retardation Factors (R) and Parameters Used to Calculate Retardation Factors:
  - Aquifer Matrix Bulk Density (ρ_b)
  - Adsorption Coefficient
    - Fraction of Organic Carbon (f_{oc})
    - Normalized Distribution Coefficient for Organic Carbon (K_{oc}),
- Dissolved Plume Solute Half-Life ($t_{1/2}$)
- First Order Chemical Decay Coefficients (λ)
- Dispersion Coefficients (α_x, $\alpha_{y,\text{ and }}$ α_z)
- pH

6.6 Baseline Stresses

Baseline stresses are currently operating influences on the hydrogeologic system and can include anthropogenic influences. Baseline stresses may include, but are not limited to:

- Contamination Concentrations
- Source Loading of Contaminants
- Groundwater Pumping or Injection
- Natural or Man Induced Recharge
- Hydraulic Barriers
- Groundwater Interaction with Surface Waters
- Underground Utilities, Structures, Tunnels, and Drainage

Baseline stresses may be constant over time or may change. Values of baseline stresses on the hydrogeological system within the modeled area can also be manipulated during calibration in an attempt to match predicted values from calibration runs with field data.

6.7 Steady State or Transient Simulations

If the model will be used for transient predictive simulations of contaminant fate and transport (*i.e.* predictive simulations that change over time), then the time steps used in the transient predictive simulations should be sufficient to obtain accurate iterative solutions and to adequately simulate variations of contaminant concentrations over time. The model should also simulate maximum possible contaminant concentrations at point of demonstration wells and other pertinent possible receptors. A steady state model can be used if the objective of modeling is to predict what the maximum contaminant concentration may be at the point of interest, regardless of how long it takes the maximum concentration to occur. Steady state modeling should be done in a way to predict the maximum plume concentration. A transient model can be used if the objective of modeling is to predict how long it may take a maximum concentration to occur at a specified location.

7.0 MODEL CALIBRATION

Calibration consists of changing values of model input parameters so that simulated values match measured values within acceptable and pre-established calibration criteria.

7.1 Method of Model Calibration

Calibration should proceed by first changing those parameters with the lowest level of accuracy, and then fine-tuning the simulation by adjusting other parameters. Typically, the model parameters with the greatest uncertainty, including those that are not easily measured or can have significant spatial variability, are used for initial adjustment in calibration. Complexity of the parameter adjustments should increase slowly. Parameters should be adjusted within a reasonable, limited range relative to field measured or literature values or both. Criteria for an acceptable calibration can be defined in a quality assurance plan. The rationale and assumptions used to adjust hydrogeological parameters during calibration should be presented in the modeling report. 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.

The model calibration method should include:

- Setting pre-simulation calibration targets and criteria from which to judge the acceptability of the calibration
- Performing the calibration process
- Evaluating the level of calibration based on the stated targets and criteria

The objective of the calibration process is to obtain acceptable agreement between model calculated values and corresponding measured values. The calibration process systematically varies model parameters within predetermined ranges based on site data and professional judgment to obtain this agreement.

Since the goodness-of-fit of the model is defined by comparing simulated values to corresponding measured values, a quantitative measure of this fit needs to be developed. This measure is defined as an objective function.

The overall model calibration process can be conducted in three steps:

- Calibration to a representative steady-state period
- Calibration to a representative transient period
- Verification of calibration to the full study period

The calibration process can proceed by first approximating model parameters using a steady state calibration period. The model parameters from the steady-state calibration can then be used as initial estimates for the transient calibration period to refine the model. Finally, the calibrated model can be run over the entire study period to verify that acceptable agreement between the model and field data has been reached.

In the steady-state mode, all the model parameters are fixed and do not vary with time. Annual averaged groundwater levels can be used or approximated. Simulated contaminant concentrations can be compared to measured concentrations in a stabilized plume. In the transient calibration, the model output for various time steps can be compared to measured time-series values, such as water levels that vary monthly, seasonally, or during the course of a pumping test, and time-series contaminant concentrations of groundwater samples.

The calibration can be done manually or automated. Manual “trial and error” calibration involves making small changes to the input files, running the model, and assessing the improvements made in matching simulated values to corresponding measured values. For numerical models this may include matching hydraulic heads, hydraulic gradients, streamflow gains and losses, water mass balance, contaminant concentrations, contaminant migration, and contaminant degradation. For analytical models this may include matching seepage velocities and contaminant concentrations.

Trial and error calibration can be time consuming, but it allows the modeler to inject knowledge and understanding of the hydrogeological system into the calibration process. In trial and error calibration, modelers have the ability to continuously change the conceptualization of the system and parameter distributions in order to improve the calibration. The insight and skill of the modeler during a trial and error calibration can control how well a model represents the groundwater system under investigation. In evaluating the adequacy of a model calibration, the conceptual model and the insight of the modeler can be as important as evaluation of quantitative measures of goodness of fit.

A recent development is the automated estimation of parameters by computer algorithms that will optimize the calibration of models. These techniques are based on minimizing an objective function. The larger the computed objective function is, the greater the discrepancy between simulated values and corresponding measured values. A key concept in automatic parameter estimation methods is that a limited set of parameters used in the model is designated to be automatically adjusted. These parameters usually are identified for specific regions of the model that are determined before the calibration process. The parameters and boundary conditions that are not identified for automatic calibration either remain fixed at their initial values or must be calibrated by trial and error.

Automated calibration techniques will find the optimal set of parameter values that result in a minimal value of the objective function. Such techniques can save a modeler time in the calibration process. A drawback to automated calibration is that a computer algorithm only knows as much about the hydrogeological system as the modeler is able to tell it. Sometimes the computer algorithm can move too far from known data in an effort to closely match measured values. The automated techniques can yield unreasonable results if insufficient constraints are supplied.

Contaminant transport models require that the groundwater flow field first be evaluated. Groundwater transport model calibration will require a minimum of two discreet sampling events from an appropriate time interval from the site. Calibrating a groundwater transport model using too few sampling events, or sampling events at short time intervals, can lead to serious errors in predictive calculations. The modeling report must justify the field data used to calibrate a contaminant transport model.

The modeler should avoid the temptation of adjusting model input data on a scale that is smaller than the distribution of field data. This process, referred to as "over calibration", can result in a model that appears to be calibrated but has been based on a dataset that is not supported by field data.

A groundwater model may inadequately assess model calibration. This deficiency may be due to the absence of clearly stated calibration targets and a failure to quantitatively assess the level of calibration achieved. Two common problems are strong indicators of model error:

- The model does a poor job of matching observations
- The optimized parameter values are unrealistic and confidence intervals on the optimized values do not include reasonable values

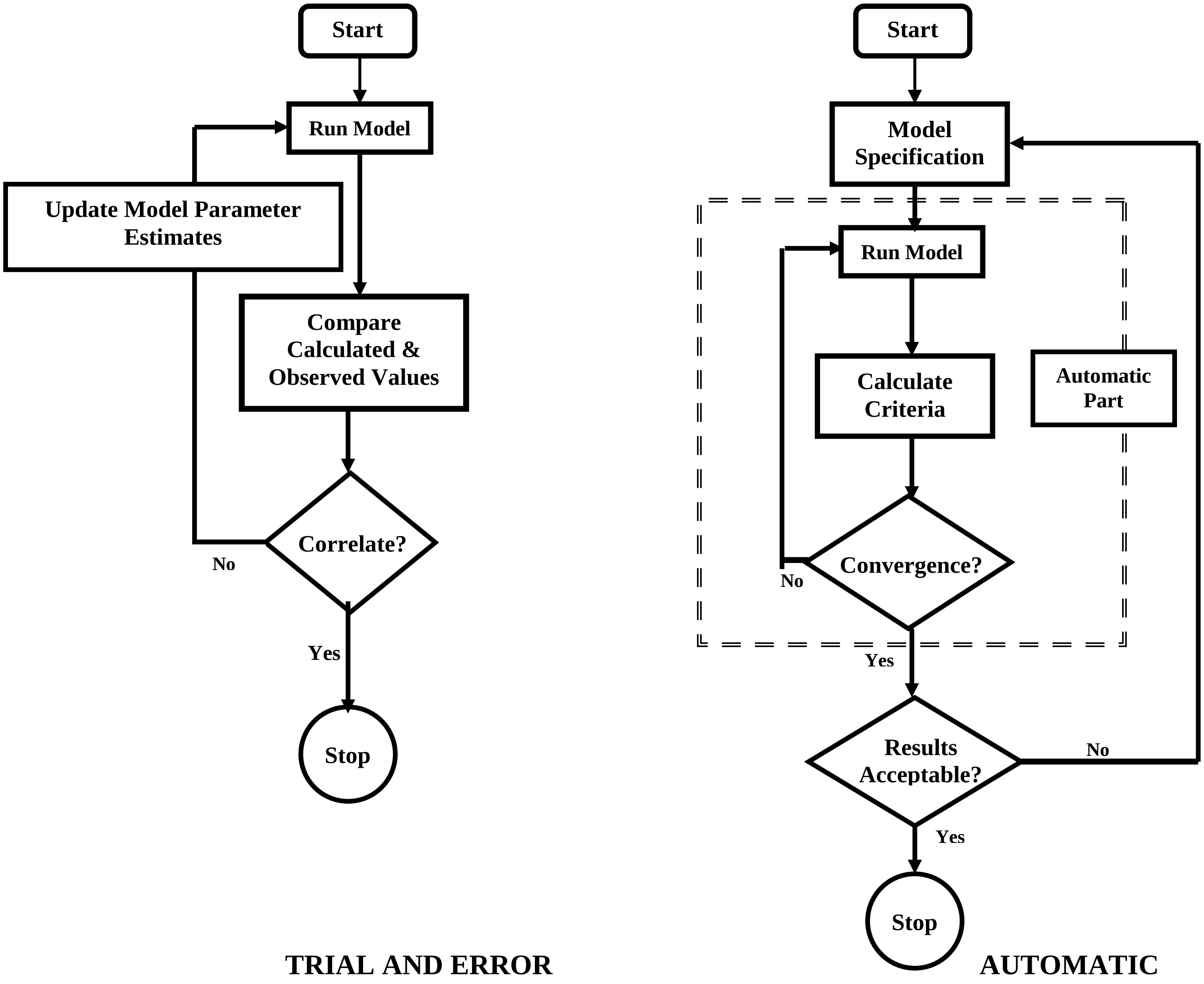

Figure 7-1: History Matching/Calibration Using "Trial and Error" and Automatic Procedures. [*Modified from van der Heijde, et. al. (1988) after Mercer and Faust (1981).*]

The level of model calibration should be defined:

- Level 1: Simulated value falls within target (highest degree of calibration).
- Level 2: Simulated value falls within two times the calibration criterion.
- Level 3: Simulated value falls within three times the calibration criterion.
- Level N: Simulated value falls within N times the calibration criterion (lowest degree of calibration).

Just because a model is calibrated does not ensure that it is an accurate representation of the hydrogeological system. The appropriateness of the conceptual model of the hydrogeological system is frequently more important than achieving the smallest differences between simulated and measured values. If a groundwater model is to have credibility it must respect what is known about the system hydrogeology. While the measures of calibration might make a model appear to be well-calibrated, the violation of a reasonable conceptual model may make the model a poor model. During model calibration the conceptual model of the hydrogeological system should be evaluated and adjusted as needed.

A model developed according to a well-argued conceptual model with minor adjustments may be superior to a model that has smaller discrepancies between simulated values and corresponding measured values resulting from unjustified manipulation of the parameter values. 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 modeling report must document the level of calibration achieved for the model. Documentation of the calibration should include listing of the calibration targets, number of nodes used for calibration, objective functions for calibration targets, and the percentage of the total number of simulated values falling within an objective function. This information should be presented in the report at least in tabular form. The distribution of the levels of calibration should be shown graphically in map form in the modeling report.

7.2 Calibration Targets

A calibrated model simulates historical conditions within an acceptable range of uncertainty, which needs to be defined before the model is calibrated. A groundwater model can be calibrated by comparing simulated values with corresponding measured values. The measured values used for comparison against simulated values are termed calibration targets.

Calibration targets are defined in terms of the type of measurement, its location and date of measurement, and measurement value. An objective function is a measure of the fit between simulated values and corresponding measured values. The model parameters modified during calibration are typically those that have the largest uncertainty and impact the objective function value as they are varied.

Different calibration targets would be used for calibration of analytical and numerical models. For some analytical models, calibration targets may be limited to groundwater seepage velocities and contaminant concentrations. For numerical models calibration targets can include the following:

- Steady state or transient hydraulic heads
- Groundwater-flow direction
- Hydraulic gradient
- Water mass balance
- Streamflows
- Streamflow gains and losses
- Contaminant concentrations
- Contaminant migration rates
- Contaminant migration directions
- Contaminant degradation rates
- Contaminant mass balance

The calibration data set should include measurements over the lateral and vertical extent of the model area. For a flow model these data will often consist of water level measurements from monitoring wells and piezometers. Contaminant concentrations measured in groundwater samples can be used to calibrate a contaminant transport model.

The relative importance of the calibration targets can be incorporated through weighting factors assigned to each class of calibration targets. The weighting factors should represent an estimate of the measurement error for each calibration target. Errors must be an estimate of the underlying accuracies of the measurements and not a measure of variation in the measurements over time. Weighting factors can be applied to account for factors such as clustering of observations in time or space.

In the case where parameters are well characterized by field measurements, the range over which that parameter is varied in the model should be consistent with the range observed in the field. The calibration target size may be too large and/or the number of targets too few or poorly distributed, thereby introducing additional uncertainty into the model results. Using multiple calibration targets increases the confidence that the model accurately represents the stresses imposed on it.

7.3 Calibration Criteria and Quantitation of Calibration

Calibration is evaluated by analyzing the residuals, or differences between simulated values and corresponding measured values, at specific locations and times. Criteria for achieving and documenting model calibration can be established in a quality assurance plan.

The degree of fit between model simulations and field measurements is the objective function which can be quantified by statistical means. Prior to calibration of the model, appropriate calibration targets should be selected from the available field data. The calibration criteria must be defined along with the rationale for establishing when a model is calibrated, and when calibration efforts should be terminated.

Calibration is by its nature non-unique. Many combinations of model parameters may result in a model that fits the field data. The modeling report must justify the model parameters used in the calibrated model. It is best if the parameters are consistent with measured or literature values or both. If model parameters used in the calibrated model are not consistent with measured or literature values, the modeling report must document how the use of these parameters may compromise the usefulness of the model.

Model calibration is evaluated by considering the magnitude of the residuals and their distribution both statistically and relative to independent variable values such as location and time. There are different quantitative criteria that can be used to demonstrate calibration of a steady-state or transient groundwater model. These may include:

- All hydraulic head residuals are within a pre-established range.
- The average and standard deviation of hydraulic head residuals is below a pre-established value.
- Average and standard deviations of head-dependent boundary flow residuals are below pre-established values.
- Magnitudes and directions of hydraulic head gradient residuals are within a pre-established range.
- All residuals of hydraulic heads between model layers are within a pre-established range.
- Average and standard deviations of residuals of hydraulic heads between model layers are below pre-established values.
- The number of flooded and dry cells within the model domain will be less than a defined percent of the model cells in the active model domain and will be randomly distributed.
- All streamflow and streamflow gain and loss residuals are within a pre-established range.
- Average and standard deviations of streamflow and streamflow gain and loss residuals are below pre-established values.
- Mass balance of the groundwater flow into and out of the modeled system is below a pre-established error value.

- All contaminant concentration residuals are within a pre-established range.
- The average and standard deviation of contaminant concentration residuals is below a pre-established value.

In initial model runs, large residuals or a bias in the distribution of residuals can indicate gross errors in the model, the data, or how values were simulated. For steady-state simulations, residuals would be calculated for specific locations within the model domain. For transient simulations residuals would be calculated for specific locations within the model domain at specific times.

The areal distribution of residuals is also important to determine whether some areas of the model are biased either too high or too low. Positive and negative residuals for hydraulic head, groundwater flow, contaminant concentration, and other calibration targets should be randomly distributed on a geographic and temporal basis.

The objective functions define the acceptable differences between the measured and simulated values for each calibration target. Documenting the degree of model calibration is important since it helps demonstrate how well the model estimates reality. Comparisons between simulated values and corresponding measured values should be presented in maps, tables, or graphs. Locations of point measurements used to set calibration targets should be presented in map form to illustrate the relative locations of targets and nodes. Ideally, a selected calibration value should be measured at a large number of locations, uniformly distributed over the modeled region, and have small associated error.

Hydraulic head measurements or contaminant concentrations can be presented in the form of contour maps and cross sections of observed and simulated values. The general shape of the calibrated potentiometric surface should be similar to observed site conditions including mounds, depressions, and general flow directions. A mass balance of water flow and contaminant mass should be presented for the calibrated model.

Statistical evaluations of residuals should be presented in tabular and graphical formats. An x-y scatter plot of observed versus simulated heads will show the magnitude and bias in residuals. An example of such a plot is shown in Figure 7-2.

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 simulations and measured field conditions. For instance, a criterion for calibration may be that residuals are is less than 10 percent of the variability in the field data across the model domain.

Measures of model calibration can be expressed as lumped parameters such as the mean of the absolute value of the differences, root mean square, absolute value of the mean differences, or the mean difference between simulated and measured values. While easy to calculate, lumped parameters are only a gross indication of the calibration because they hide poorly calibrated portions of the model *via* the averaging process. Lumped parameters may give no indication of the spatial variability of calibration results, and therefore should not be used as the only demonstration of model calibration.

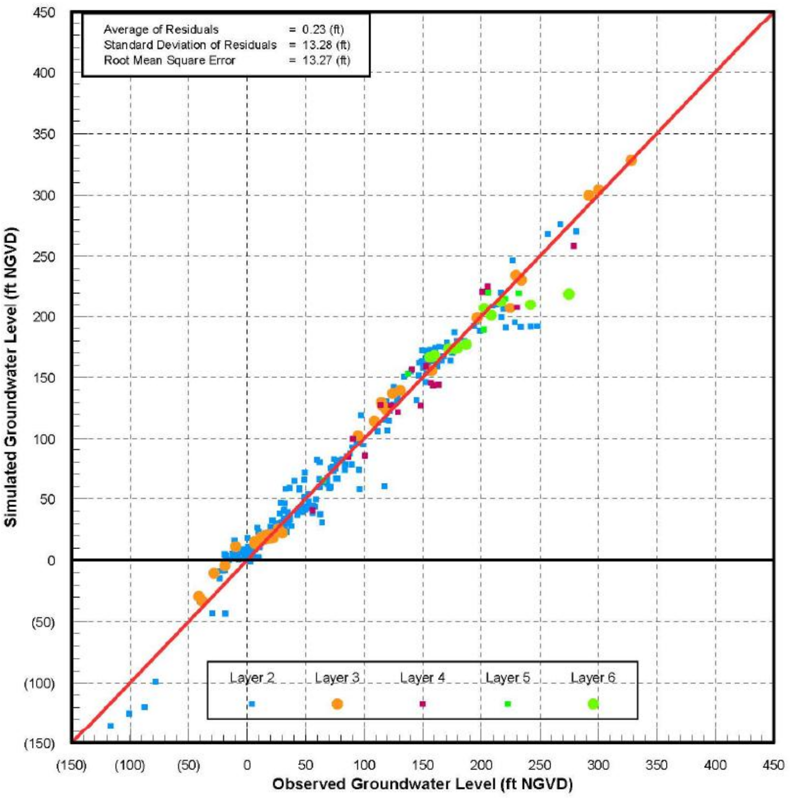

Figure 7-2: Residual Scatter Plot Example

7.4 Degree of Model Calibration

There can be three basic applications of a groundwater model:

- Predictive simulations of groundwater flow and contaminant transport
- Interpretative simulations used as a framework for studying dynamics of the hydrogeological system, identifying data gaps, and planning field data collection efforts
- Generic simulations used to interpret hypothetical conditions of the hydrogeological system

For predictive simulations to be acceptable the groundwater model must be calibrated and calibration of the model must be documented in the modeling report. Interpretative simulations do not necessarily require model calibration and generic simulations can be done when there are no comparative data for model calibration. It may be possible to use un-calibrated numerical or analytical models for interpretative or generic simulations, but not for acceptable predictive simulations.

Numerical groundwater flow and contaminant transport models can usually be calibrated sufficiently to use for acceptable predictive simulations. It may be more difficult to calibrate analytical models due to the limited number of model parameters that can be adjusted to achieve calibration. It may be possible to calibrate an analytical model of a linear groundwater flow system, with relatively short flow paths, in a single-layer aquifer with homogenous aquifer properties and consistent contaminant source concentration and transport properties under steady-state conditions. It may be difficult to calibrate an analytical model of a non-linear groundwater flow system with longer flow paths in a single- or multi-layer aquifer with varying aquifer properties, contaminant concentrations, or contaminant transport properties.

It may not be possible to calibrate a groundwater model because of:

- The type of model developed (analytical versus numerical)
- The complexity of the model (model layers, model dimensions, heterogeneity of hydraulic and contaminant concentration or transport properties, steady-state versus transient capabilities)
- Inadequacy of the conceptual site model
- Insufficient data for model calibration
- A lack of time or project budget for model calibration

If, for any reason, a groundwater model cannot be calibrated, the modeling report must demonstrate that predictive simulations made with the un-calibrated model were sufficiently conservative to allow the modeling results to be used to meet project objectives.

Overly conservative estimates of groundwater flow or contaminant transport may result in higher costs for remedial action scenarios to meet compliance or clean up objectives. Refinement of a groundwater model may avoid such overly conservative estimates. A model may be refined by:

- Using a numerical rather than an analytical model
- Developing a more complex model to accommodate complexities or temporal variations in the hydrogeological system
- Collection of sufficient site-specific data to refine the CSM and to allow for adequate model calibration
- Running transient rather than steady-state simulations
- Allowing sufficient time and project budget for model calibration

In some situations the cost of refining a groundwater model may be a fraction of the cost needed to deal with overly conservative estimates of groundwater flow or contaminant transport.

7.5 Calibration of Analytical Models

The preceding details of Section 7.0 apply best to calibration of sophisticated numerical models. Some of the details can apply to an analytical model, but most analytical models do not have the same or as many aspects of model construction, model input parameters, and boundary conditions with which to make calibration adjustments. It is often said that an analytical model does not have as many “calibration dials” as a numerical model.

Some of the calibration methods described in the section can be applied to an analytical model, but this depends on how many and what types of calibration dials are available in the analytical model. Calibration of an analytical model must be designed based on the available calibration dials.

For instance, the analytical code BIOCHLOR, developed by AFCEE and available on the CSMoS website allows for input of single values of aquifer hydraulic conductivity, hydraulic gradient, aquifer porosity, dispersivity, soil bulk density, and fraction organic carbon. First-order decay coefficients can be specified for two zones within the modeled domain. BIOCHLOR does not allow for multiple aquifers, specification of aquifer thickness and geometry, varying aquifer properties, boundary conditions, recharge, surface water-groundwater interactions, or transient conditions. While a model developed using BIOCHLOR cannot be calibrated to measured hydraulic heads, it could be calibrated by adjusting the input parameters until simulated constituent concentrations reasonably match measured concentrations.

Because of the limited number of calibration dials in an analytical model such as BIOCHLOR, it may not be possible to reasonably adjust input parameters so that simulated constituent concentrations reasonably match measured concentrations. In this case, use of a more sophisticated numerical model with more calibration dials should be considered.

The analytic element modeling (AEM) module of the Groundwater Modeling System (GMS) graphical user interface for MODFLOW allows for specification of more input parameters than BIOCHLOR such as specified head boundaries, aquifer thickness, rivers, recharge, and production wells. The AEM software is limited to single-layer, steady-state models so there may still be limitations in fully depicting a CSM. However, an AEM model can have more calibration dials than a BIOCHLOR model.

Section 7.3 presented information on quantitation of calibration. Because output is limited for some analytical models, quantitation of calibration can be difficult. However, even in an analytical BIOCHLOR model, quantitative comparisons can be made between simulated and measured constituent concentrations. In an AEM model simulated hydraulic heads and stream flows can be quantitatively compared to measured hydraulic heads and stream flows. Consequently, quantitative metrics of calibration residuals can reflect limitations in output from analytical models.

If an analytical model cannot be calibrated to the degree described in this section the modeling report must document that calibration, to the degree it was completed, was sufficient to meet the modeling objectives. Documentation of calibration can include, but may not necessarily be limited to:

- Comparison of simulated concentrations at specific locations to measured concentrations at the same locations (e.g. such as could be done with BIOCHLOR or BIOSCREEN).
- Comparison of simulated hydraulic heads and water fluxes to measured hydraulic heads and water fluxes (e.g. such as could be done with GMS AEM and Visual AEM).
- Comparison of simulated recovery well capture zones to measured recovery well capture zones (*e.g.*, such as could be done with WHAem).
- Comparison of simulated groundwater concentrations resulting from soil leaching to measured groundwater concentrations between leaching areas (e.g. such as could be done with VLEACH or SESOIL).

With an analytical model with limited calibration dials, conservative simulations (*i.e.*, overestimating the rate or extent of constituent movement) can sometimes be run in *lieu* of developing a more complex model with more calibration dials. Documentation of matches between simulated and measured parameters should be done graphically (by means of comparing model output to maps of hydraulic heads or contaminant concentrations) or in tables.

8.0 DATA SENSITIVITY ANALYSIS

Sensitivity analysis is performed to determine the relative impact of changes in model input parameters on model output. Some input parameters are more important in determining model outcome than other parameters. Their relative importance can be influenced by site-specific conditions and the properties of the contaminants being modeled. Sensitivity analysis can also be used to help quantify the uncertainty in model prediction due to uncertainty in an input parameter. For example, if a potentially sensitive parameter is varied over an expected range of possible values, a range of model outcomes is produced, and inferences can be made about uncertainty in the model predictions due to uncertainty in that parameter. For example: f_{oc} can be a sensitive parameter when modeling the fate and transport of organic contaminants as shown in Appendix A in the example using BIOCHLOR. The modeler is also able to select values from the range for use in the final model that are demonstrated to be conservative.

A model is considered sensitive to an input parameter if a small change in the parameter causes a large change in the model prediction. The sensitivity of a given parameter largely depends on its role in the governing equation of the model. However, site-specific conditions, including the properties of the contaminant being modeled, can also impact the relative importance of some input parameters, so care should be taken to perform the sensitivity analysis for a model that is calibrated for a given site rather than relying on past experience with the model at other sites.

Many input parameters used in fate and transport models actually result from analysis of an observed range of field measurements or from a range of values published in professional journals and reports, so it is clear that many model inputs are subject to uncertainty. Sensitivity analysis attempts to make clear the significance of choosing a particular value from that range of possible values for a given parameter. A procedure for using sensitivity analyses to determine how model output varies as the range of parameter values is used is presented in Foster-Wheeler (1998) and includes the following steps:

- Identify input parameters for which a range of reasonable values exists.
- Conduct model runs varying the value of the target input parameter while holding values of other input parameters constant. Vary the target input value by both increasing it and decreasing it by a small percentage or fraction.
- The number of model runs needed to determine sensitivity of an input parameter will depend on how the parameter is incorporated into the solution of the governing equation. Fewer model runs are needed if the input parameter is used in a linear form than if it is used as an exponent, raised to a power, used as a logarithm, or incorporated into a functional transformation.
- Compare model runs by calculating the percent change in the concentration predicted by the model as the target input parameters are varied to identify the most and least sensitive input parameters for the model.
- If model output is only slightly sensitive to the range of reasonable values used for an input parameter, there is generally little or no need for additional effort to better define the value. On the other hand, if model output is highly sensitive to an input parameter, it may be helpful to obtain more field or laboratory measurements of the parameter, reducing uncertainty in that parameter and consequently reducing uncertainty in the model prediction.

The relative sensitivity of model results to each tested model input parameter and boundary condition must be documented. Failure to conduct a sensitivity analysis and/or provide adequate documentation could invalidate modeling results, leading to the rejection of the entire modeling effort by EPD.

9.0 MODEL VERIFICATION AND VALIDATION

9.1 Model Verification

Model verification is a test of whether the model can be used as a predictive tool, by demonstrating that the calibrated model was an adequate representation of the physical and chemical system. The common test for verification is to run the calibrated model in predictive mode to check whether the prediction reasonably matches the observations of a reserved data set deliberately excluded from consideration during calibration.

9.2 Model Validation

Model validation is intended to ensure that the model represents and correctly reproduces the behavior of the system being modeled. Although model validation does not imply model verification, often validation is interchanged with verification since model results are usually compared to measured data from the system being modeled. If model results are proven to be insensitive to variation of input parameters that cannot be verified, a calibrated but unverified model may be used to model fate and transport of constituents[1]. The validation process consists of applying a calibrated model to a set of input parameter values and boundary conditions separate from the set used for calibration to reproduce an independent set of observations, typically the hydraulic head or solute concentrations over a different time period[2]. If a calibrated model can approximate the measurements from the represented system within an acceptable range, the model is validated as a satisfactory representation of the system.

Depending on the types of models (*i.e*. analytical model and numerical model), the number and extent of calculations and measurements to validate a model would be different. For example, the validation of a simple analytical model can be done by comparing model output to independent calculations using a spreadsheet. Because an analytical model will not account for field conditions that change with time or space, validation parameters for an analytical model may be more limited than those of a numerical model that is used to predict spatial and temporal changes in dissolved constituent concentrations. The validation of numerical models can be done by determining concentrations of dissolved constituents at locations where initial concentrations are not known, and by time-series sampling at locations where initial conditions are known [1]. For the model composed of a combination of independent equations, several independent calculations may be needed to validate a single model output[1]. A detailed discussion of the validation processes, assumptions, and derivations of groundwater models is beyond the scope of this document. Therefore, the reader should use and document the published references for this information.

10.0 PREDICTIVE SIMULATIONS

Upon completing calibration, sensitivity analysis, and verification of the model, can be used to predict future scenarios. Such simulations may be used to estimate:

- The hydraulic response of a hydrogeological system to changes in groundwater withdrawals, boundary conditions, and recharge
- Migration pathways of contaminants
- Contaminant retardation and decay along migration pathways
- Changes in contaminant concentrations in groundwater due to changes in contaminant source concentration or changes in contaminant mass loading rates to groundwater
- Contaminant mass removal rates as a result of remedial action scenarios
- Concentrations of a contaminant at points of compliance at future moments in time

Predictive simulations may either be run when using a model in steady-state or transient mode. In the steady-state mode all the model parameters are fixed and do not vary with time, whereas in the transient mode certain parameters such as rainfall, evapotranspiration, pumping rates, contaminant source concentrations, contaminant mass loading rates to groundwater, and other parameters are varied to generate variations in hydraulic heads or contaminant concentrations, or both. Predictive simulation conditions that are vastly different from the model calibration and validation conditions, such as high pumping rates or drawdowns, high contaminant concentrations, or vastly different contaminant retardation or decay properties, may invalidate the model as a representation of the hydrogeological system.

Predictive simulations can be:

- Groundwater flow simulations
- Contaminant transport simulations
- A combination of groundwater flow simulation and contaminant transport simulations

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[1] American Society for Testing and Materials (ASTM), 1999: RBCA Fate and Transport Models: Compendium and Selection Guidance.

[2] Michigan Department of Environmental Quality, 2002: Groundwater Modeling Guidance.

Predictive groundwater flow simulations can be run in steady-state mode, where dynamic equilibrium is achieved. Transient groundwater flow simulations can be run to simulate multiple time periods when stresses on the aquifer such as groundwater withdrawals, boundary conditions, and recharge may change.

Predictive contaminant transport simulations may be run until the contaminant plume has reached steady-state (or near steady-state) conditions. Assuming the source and mass loading of the contaminant to groundwater remains constant (or near constant), at some moment in time the contaminant plume will reach a maximum size and the shape of the plume will remain relatively fixed for future times. Running steady-state contaminant transport simulations requires running the groundwater flow simulation in steady-state mode using average hydrogeological conditions. Because the time span of groundwater contaminant travel is usually measured in years, over the span of multiple years the seasonal groundwater flow variations can be averaged out so that performing transport models with a transient groundwater flow model may not be required.

Transient contaminant transport predictive simulations should be used *if* there will be noteworthy changes in groundwater withdrawals, model boundary conditions, or recharge, *or* changes (increases or decreases) in contaminant source concentrations or mass loading rates to groundwater. Transient contaminant transport predictive simulations can also be used to predict the effects of remedial action scenarios on groundwater flow and contaminant concentrations.

Transient numerical simulations would allow aquifer stresses and contaminant source concentrations and mass loading rates to be varied over time. Analytical models typically cannot accommodate temporal variation of parameter inputs. Analytical models require input of specific hydraulic properties, aquifer stresses, contaminant concentrations, contaminant transport properties such as retardation and decay rates, and a simulation time for each individual simulation. Model inputs can be varied incrementally for a series of individual simulations to generate pseudo-transient groundwater flow and contaminant transport simulations.

Pseudo-transient contaminant transport simulations may grossly over- or under-predict groundwater flow or contaminant transport or both. Pseudo-transient simulations should therefore not be used if there may be noteworthy temporal changes to groundwater flow or contaminant source or transport conditions. In such situations, transient numerical simulations would better predict groundwater flow and contaminant transport and would be more likely to achieve modeling objectives. Predictions generated using numerical simulations may also result in lower costs for remedial action scenarios needed to achieve compliance or cleanup goals.

If pseudo-transient analytical models are used to simulate groundwater flow and contaminant transport over varying time intervals, the modeling report must demonstrate that pseudo-transient simulations do not incorrectly predict groundwater movement or under predict contaminant concentrations at modeled locations and time intervals.

Predictive simulations should be viewed as estimates and not as certainties. There is always some uncertainty in predictive models. The simulations are based on the conceptual model, the hydrogeological and contaminant 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.

Time periods over which a model is calibrated may be small compared to the length of time used for predictive simulations. Relatively small errors observed during the time period over the model calibration may be greatly magnified during predictive simulations because of the larger time periods used in predictive simulations. The growth in errors resulting from projecting model simulations 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.

11.0 UNCERTAINTY OF MODEL PREDICTIONS

The response of the model to various prediction scenarios should be presented in both narrative and graphical forms. Model predictions should be expressed as a range of possible outcomes, which reflect the uncertainty in model parameter values. The range of uncertainty should be similar to that used for the sensitivity analysis. Expression of model predictions as ranges is illustrated in Figure 11-1.

Predictive simulations may be conservative. That is, given the uncertainty in model input parameters and the corresponding uncertainty, model input values may be selected that result in a "worst-case" simulation. Site-specific data may be used to support more realistic predictive simulations. Site-specific data can be collected to limit the range of uncertainty in predictive simulations and to minimize the conservativeness of such simulations.

The cost of site-specific data collection may be a fraction of the cost of remedial action scenarios needed to deal with overly conservative estimates of groundwater flow or contaminant transport. In situations where long-term remedial action may be necessary, it may be useful to refine and update predictive simulations as additional data are collected and future aquifer stresses or contaminant source concentrations and mass loading rates are observed.

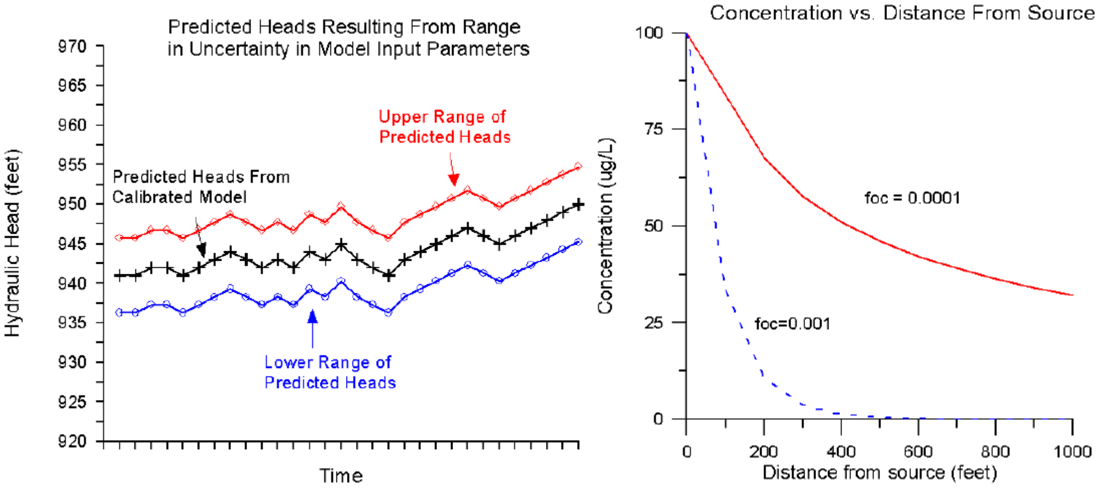

Figure 11-1 Examples of Graphical Representations of Ranges of Model Predictions

If a model was not adequately calibrated or verified, or the complexity of the model would not allow adequate calibration and verification, it must be documented that predictive simulations made with the model were sufficiently conservative (*i.e.*, tend to over-estimate rather than under-estimate contaminant migration) to allow the modeling results to be used.

12.0 PERFORMANCE/POST AUDIT MONITORING AND MODEL REFINEMENT

Groundwater models can be useful tools in simulating hydrogeologic conditions and contaminant concentrations over time. However, small errors in the predictive model may result in large errors when projected forward in time. Performance monitoring is required to compare future conditions with modeled conditions and assess errors in the model. Depending on purpose of the model, and accuracy of the parameters used for simulation, an effective performance-monitoring plan, with submittal of regularly scheduled progress/performance reports, must be developed.

Errors in groundwater models become evident with the collection of additional data from effective performance monitoring. As additional data becomes available, the model should be refined to more accurately predict future conditions. The refined predictive model should be rerun based on the additional data and any changes to the original predictive model should be discussed in the appropriate progress/performance monitoring reports. A performance/post audit monitoring plan should be provided.

Some common Modeling Errors to Avoid include, but are not limited to:

- Units are inconsistent (For example, using standard and metric units without converting)
- Insufficient field data for calibration
- Insufficient boundary size and/or conditions
- Inaccurate hydrologic assumptions
- Incorrect sign for pumping or recharge
- Typographical errors or general mistakes in input values
- Using unrealistic input data that doesn't match the site
- Excluding data from wells with the highest contamination
- Improper selection and use of source and target wells
- Target wells clustered in only a small portion of the model
- Incorrect assumptions regarding the effect of soil/source removal on source area groundwater contamination. For example, assuming a 50% contamination loss in source well due to removal of overlying soil.
- Forcing data to fit using maximum or minimum ranges of input values
- Acceptance of model output without logical assessment

13.0 MODELING REPORTING REQUIREMENTS

Submittal of a stand-alone report, which may be included as an appendix to another submittal, as support documentation, to EPD will be required for all facilities requesting approval of groundwater modeling results. The report must be an all-encompassing document that contains enough information to allow EPD to duplicate the model if EPD finds that such an effort is necessary. This may require providing EPD with model input files and a table summarizing the input parameter values, the source/justification of these values, and sufficient output sheets to verify modeling objectives have been met. Appendix B provides two examples of such tables for BIOCHLOR and BIOSCREEN.

A groundwater modeling report must contain the following at a minimum:

- A general description of the mode.
- A demonstration that the model is appropriate
- A description of the scope of the model
- A description of the site environmental history
- A description of current groundwater conditions
- A list/table of model input values and their source/justification
- Any input values that are neither site-specific values *nor* reference values must be proven to be conservative
- A description of model calibration procedures
- A description and results of a sensitivity analysis
- A discussion of model results including, but not limited to:

  - A discussion on how the plume will change through time and what to expect
  - Output data should be presented in both tabular form and a printout of the output pages should be provided
  - Supporting maps showing site details and output may provide a means of confirming the stated model objectives have been met, such as:
    - Isopleth map showing anticipated maximum extent of contaminant plume
    - Isopleth maps indicating incremental changes in plume configuration through time. Time increments should be based on the modeling objectives and correspond with proposed performance monitoring requirements
- Conclusions and recommendations for confirming the adequacy of the modeling effort or the need for additional modeling

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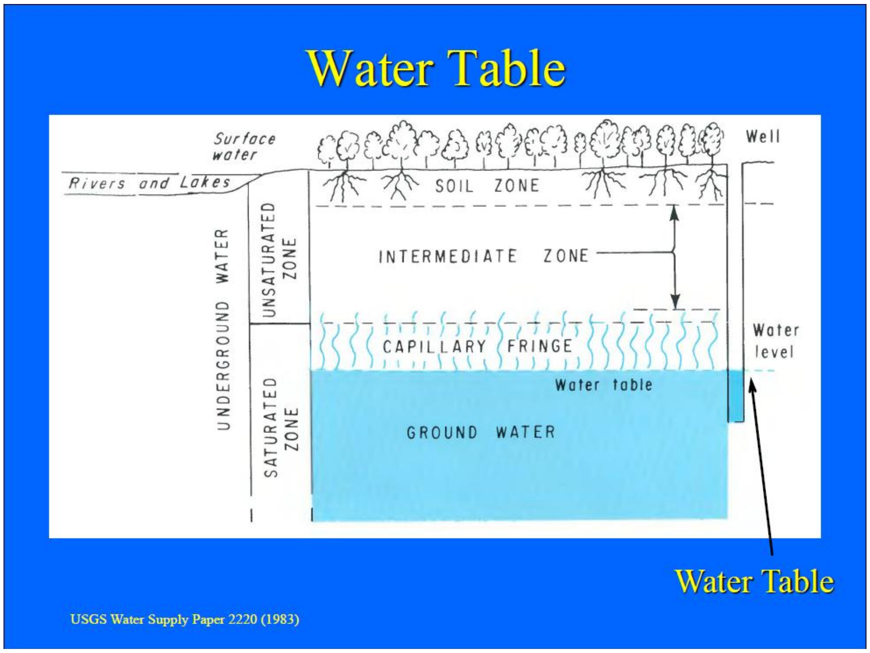
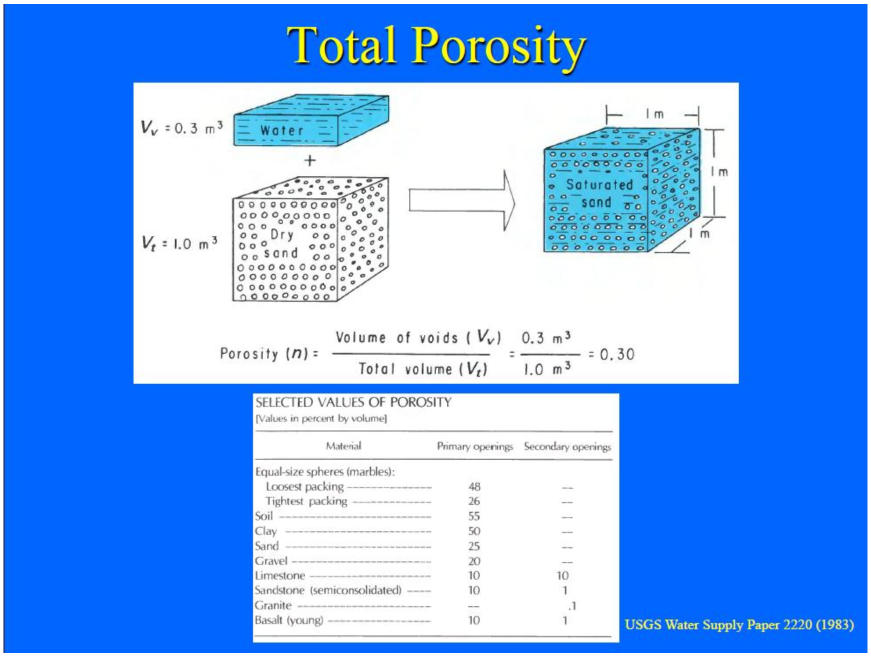
APPENDIX A: Basic Aspects of Hydrogeology



Water Table

USGS Water Supply Paper 2220 (1983)

The water table is where the hydraulic head is equal to one atmosphere. It is the level to which water will rise in a well open to the atmosphere and is below the top of the saturated capillary fringe. The top of the saturated capillary fringe is not the water table. Water in the capillary fringe is held at pressures less than one atmosphere so that capillary water cannot enter a well (*i.e.*, water will not run “uphill” from a pressure of less than one atmosphere to a pressure of one atmosphere).



Total Porosity

$$\text{Porosity } (n) = \frac{\text{Volume of voids } (V_v)}{\text{Total volume } (V_t)} = \frac{0.3 \text{ m}^3}{1.0 \text{ m}^3} = 0.30$$

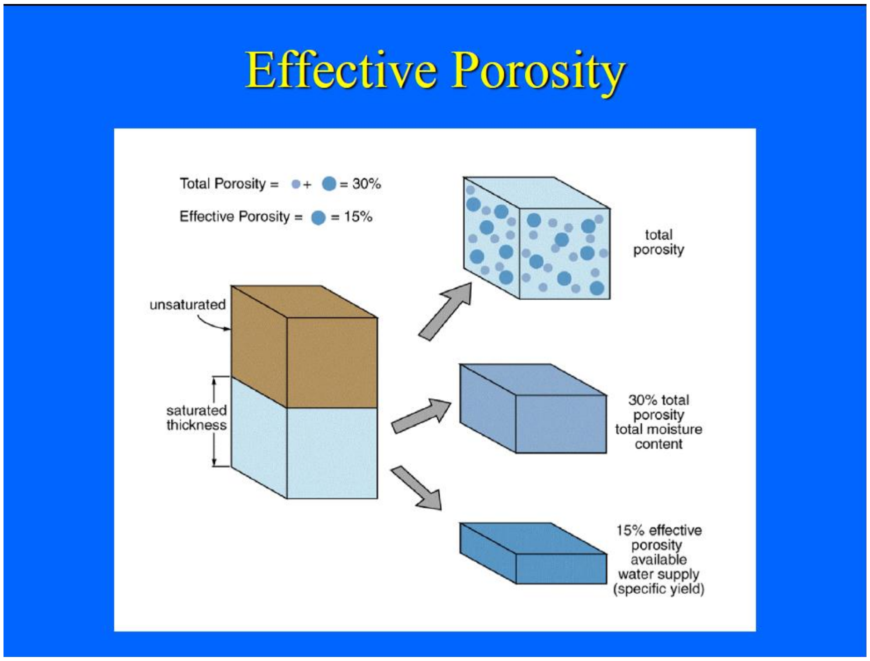
SELECTED VALUES OF POROSITY

[Values in percent by volume]

Material	Primary openings	Secondary openings
Equal-size spheres (marbles):		
Loosest packing	48	—
Tightest packing	26	—
Soil	55	—
Clay	50	—
Sand	25	—
Gravel	20	—
Limestone	10	10
Sandstone (semiconsolidated)	10	1
Granite	—	.1
Basalt (young)	10	1

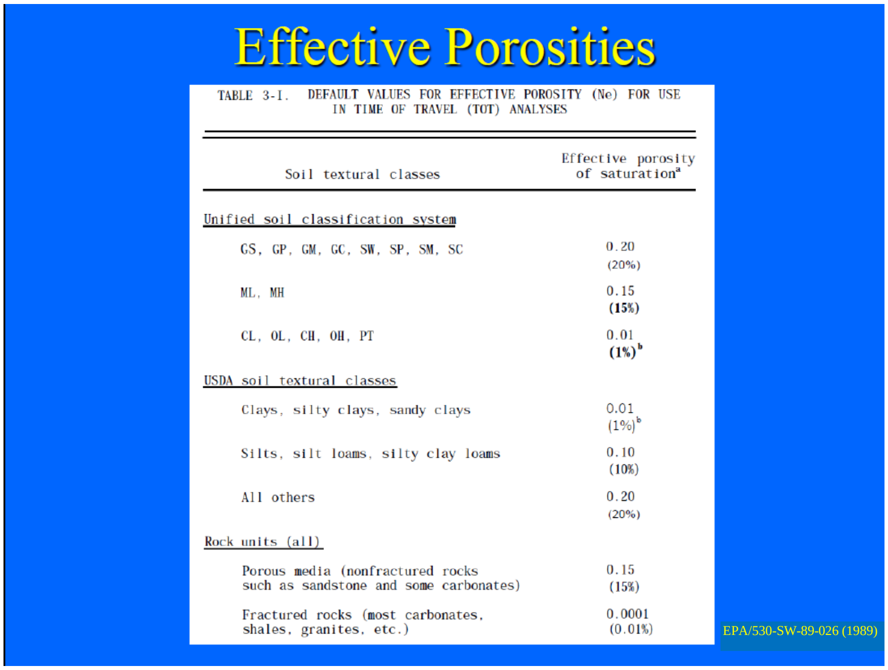
USGS Water Supply Paper 2220 (1983)

Total porosity is the ratio of openings (voids) in a soil or rock to the total volume of the soil or rock. Total porosities of fine-grained materials such as clay can be very high due to the way that individual particles are packed within the soil. Total porosities of rocks are often smaller than total porosities of soils.



Effective Porosity

Effective porosity is the porosity through which groundwater movement occurs. Effective porosity is smaller than total porosity. In coarse-grained materials such as sands and gravels effective porosity may be only slightly less than total porosity (*e.g.*, total porosity = 0.35, effective porosity = 0.30). In fine-grained materials such as silts and clays effective porosity may be much less than total porosity (*e.g.*, total porosity = 0.40, effective porosity = 0.05). Effective porosity is analogous to, but not always equal to, specific yield.



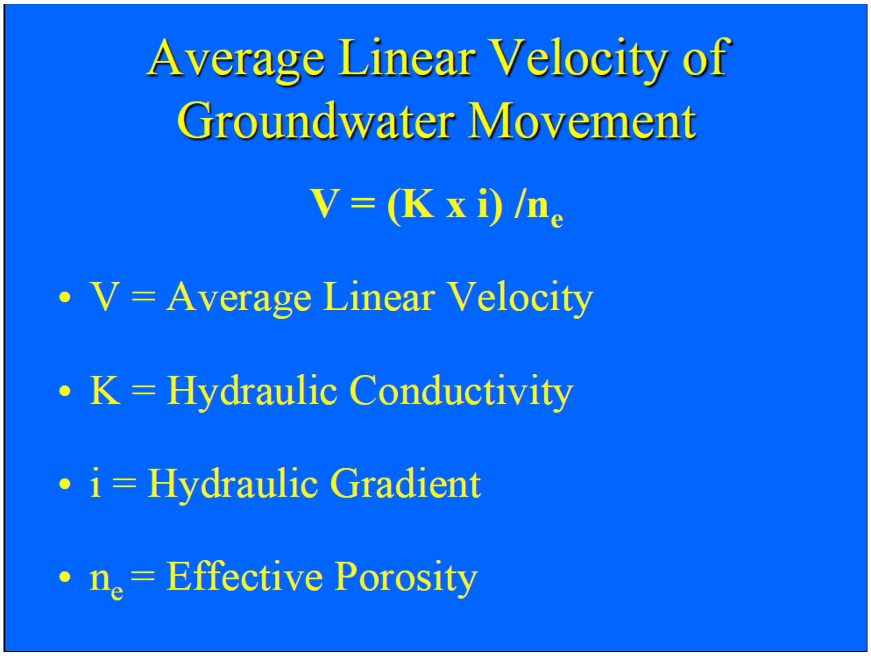
Effective Porosities

TABLE 3-I. DEFAULT VALUES FOR EFFECTIVE POROSITY (Ne) FOR USE IN TIME OF TRAVEL (TOT) ANALYSES

Soil textural classes	Effective porosity of saturation[a]
Unified soil classification system	
GS, GP, GM, GC, SW, SP, SM, SC	0.20 (20%)
ML, MH	0.15 **(15%)**
CL, OL, CH, OH, PT	0.01 **(1%)**[b]
USDA soil textural classes	
Clays, silty clays, sandy clays	0.01 (1%)[b]
Silts, silt loams, silty clay loams	0.10 (10%)
All others	0.20 (20%)
Rock units (all)	
Porous media (nonfractured rocks such as sandstone and some carbonates)	0.15 (15%)
Fractured rocks (most carbonates, shales, granites, etc.)	0.0001 (0.01%)

EPA/530-SW-89-026 (1989)

Effective porosities are related to the grain size distribution and packing of geologic materials. Finer grained materials such as silts and clays have smaller effective porosities than coarse grained materials such as sand and gravel. Effective porosities of fractured metamorphic, igneous, and sedimentary rocks can be small while effective porosities of solution-opened carbonates can be large.

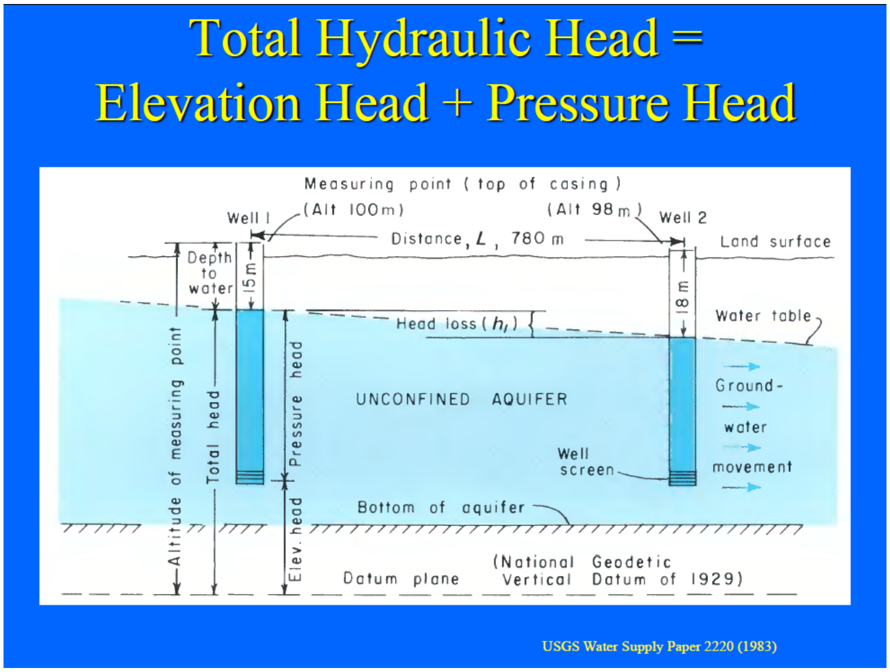


Average Linear Velocity of Groundwater Movement

$$V = (K \times i) / n_e$$

- V = Average Linear Velocity
- K = Hydraulic Conductivity
- i = Hydraulic Gradient
- n_e = Effective Porosity

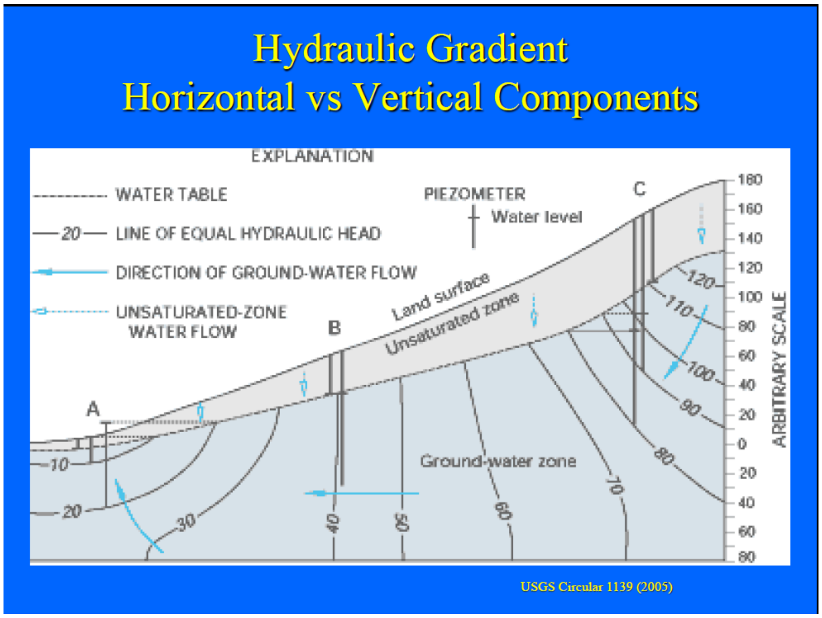
The equation for average linear velocity of groundwater movement includes hydraulic conductivity (K), hydraulic gradient (*i*), and effective porosity (n_e). With n_e in the denominator of the equation average linear velocity increases as n_e gets smaller (for a given K and *i*). For a given K and *i*, if the n_e through which groundwater can flow is smaller the groundwater must move faster through the pores to maintain the groundwater flux.



Total Hydraulic Head = Elevation Head + Pressure Head

USGS Water Supply Paper 2220 (1983)

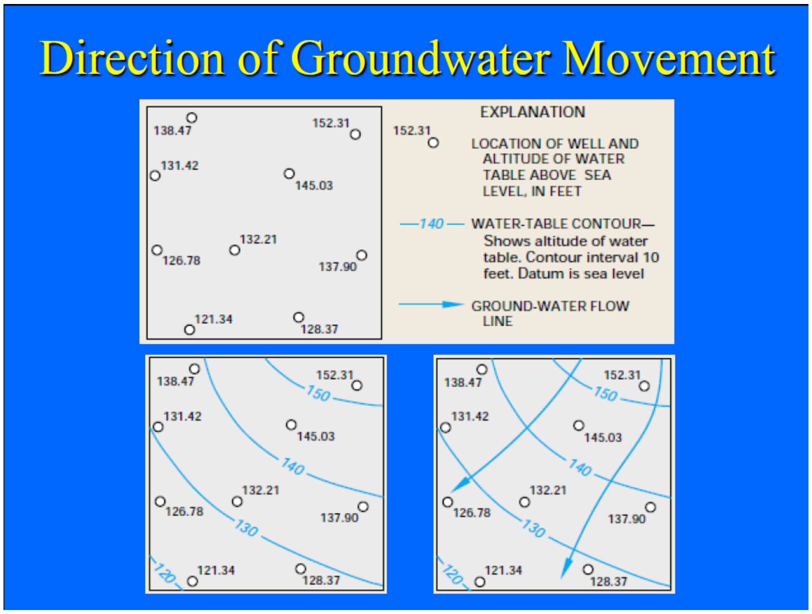
Hydraulic head is equal to elevation head + pressure head. Therefore the hydraulic head will be the same throughout the water column in a well (assuming there is no vertical component of hydraulic gradient). Hydraulic gradient is the hydraulic head loss between two wells divide by the distance between the wells (*i.e.*, hydraulic gradient; $i = \Delta h / \Delta L$).



Hydraulic Gradient Horizontal vs Vertical Components

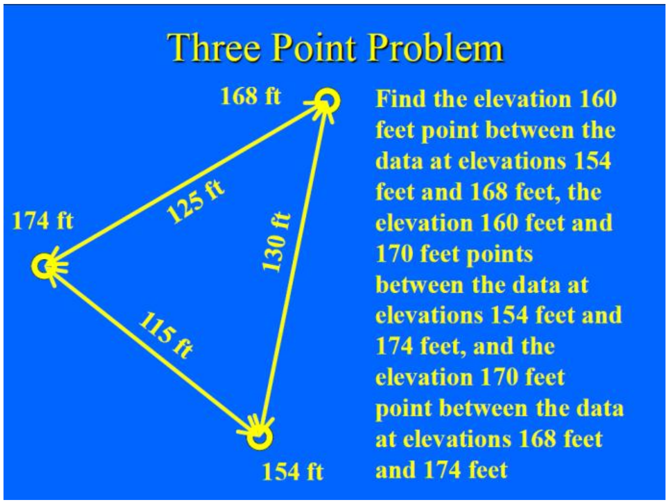
USGS Circular 1139 (2005)

Groundwater moves in all directions at the same time so that there are both horizontal and vertical components of hydraulic gradient. In groundwater recharge and discharge areas there are vertical components of hydraulic gradient. Wells close to each other in recharge and discharge areas may have different hydraulic heads that reflect the vertical component of hydraulic gradient more than the horizontal component of hydraulic gradient. Contouring the hydraulic heads of such wells would incorrectly depict the horizontal component of hydraulic gradient. Hydraulic heads between recharge and discharge areas may be hydrostatic (*i.e.*, the same at each depth in the aquifer) so that there would be no vertical component of hydraulic gradient.



Direction of Groundwater Movement

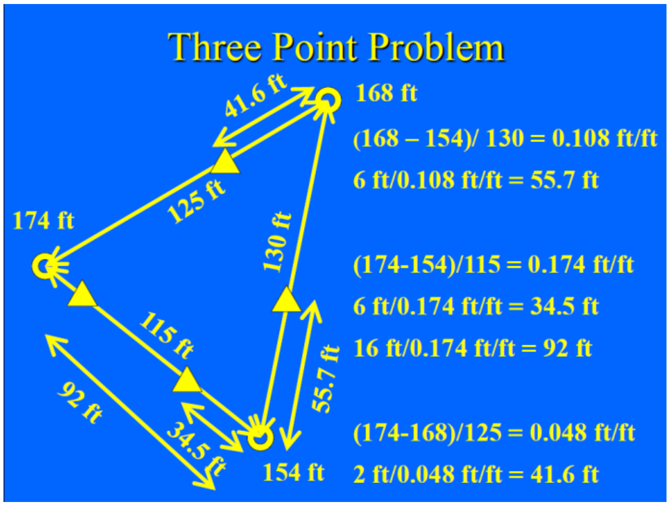
Hydraulic heads in individual wells can be contoured to generate contour lines of equal hydraulic head within the aquifer. Directions of horizontal groundwater movement are perpendicular to the hydraulic head contours. To avoid influences from vertical gradient components, hydraulic head contours should be drawn using hydraulic head data from similar portions of the aquifer (*e.g.*, shallow, middle, deep) in depictions of horizontal groundwater movement.



Three Point Problem

Find the elevation 160 feet point between the data at elevations 154 feet and 168 feet, the elevation 160 feet and 170 feet points between the data at elevations 154 feet and 174 feet, and the elevation 170 feet point between the data at elevations 168 feet and 174 feet

Three point problem solved to find the elevation 160 feet point between the data at elevations 154 feet and 168 feet, the elevation 160 feet and 170 feet points between the data at elevations 154 feet and 174 feet, and the elevation 170 feet point between the data at elevations 168 feet and 174 feet. Measure the distances between the elevation data points.



Three Point Problem

(168 – 154)/ 130 = 0.108 ft/ft

6 ft/0.108 ft/ft = 55.7 ft

(174-154)/115 = 0.174 ft/ft

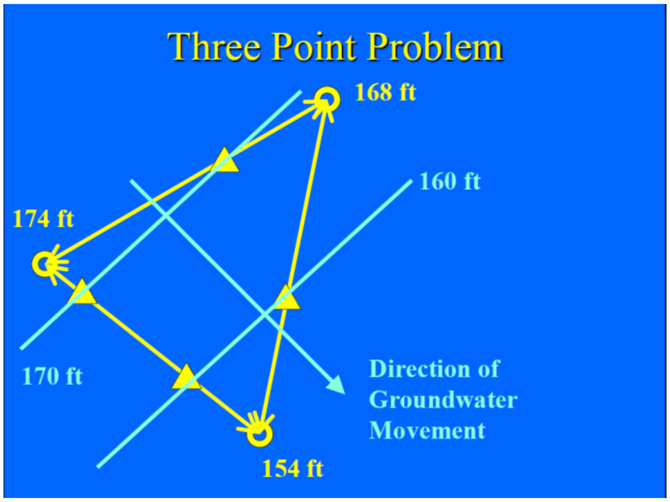
6 ft/0.174 ft/ft = 34.5 ft

16 ft/0.174 ft/ft = 92 ft

(174-168)/125 = 0.048 ft/ft

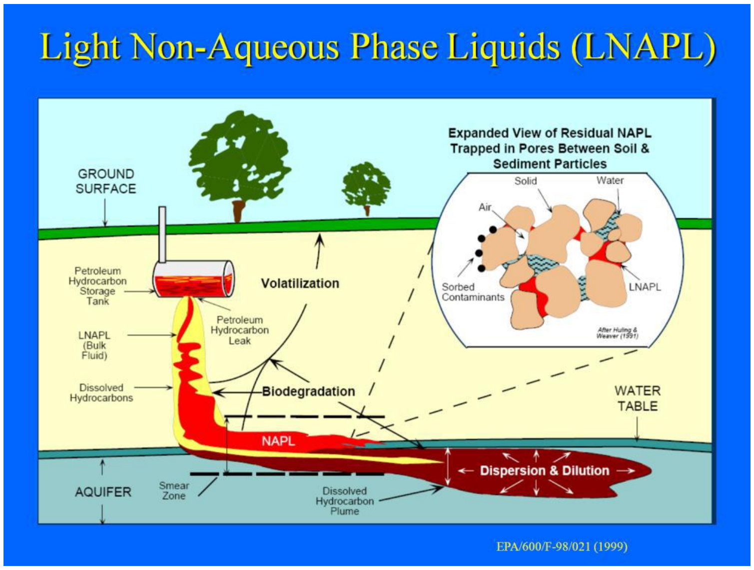
2 ft/0.048 ft/ft = 41.6 ft

Calculations are done by proportioning distances between the points of known elevation to the distances between points at elevation 154 + 6 = 160 ft., 154 + 6 = 160 ft., 154 + 16 = 170 ft., and 168 + 2 = 170 ft.



Three Point Problem

Complete the three point problem by connecting 160 feet and 170 feet data points to show groundwater contours at elevations 160 feet and 170 feet, and drawing an arrow perpendicular to the contours to show direction of groundwater movement within the area of available elevation data.



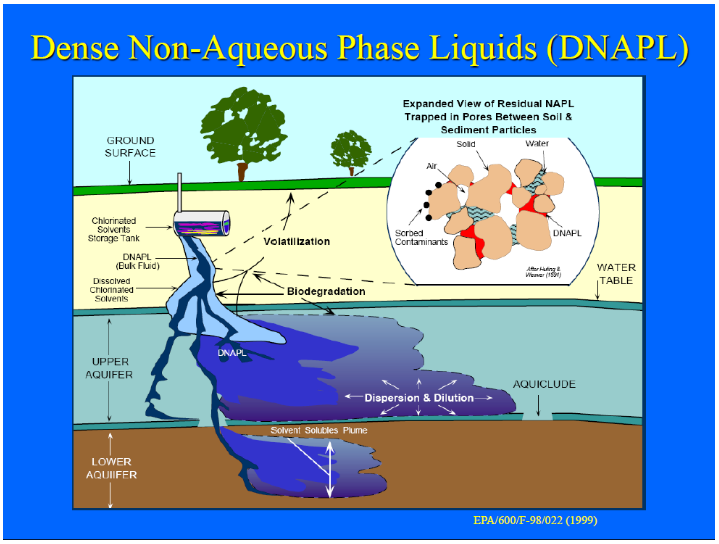
Light Non-Aqueous Phase Liquids (LNAPL)

EPA/600/F-98/021 (1999)

Light non-aqueous phase liquids (LNAPL) have densities less than water (i.e., specific gravity less than 1.00) and therefore float on the water table. Examples of LNAPL are gasoline, diesel fuel, and heating oil. LNAPLs are soluble in water to some degree. Released LNAPLs accumulate on the water table and plumes of dissolved LNAPL move downgradient of the floating LNAPL pool. In geologic materials LNAPL chemicals exist in four phases:

- Free product LNAPL
- LNAPL dissolved in groundwater
- LNAPL chemical adsorbed to organic material in the aquifer matrix
- LNAPL vapors in pore air (if there is any; typically below the water table there isn't any pore air so that the vapor phase of LNAPL does not exist)

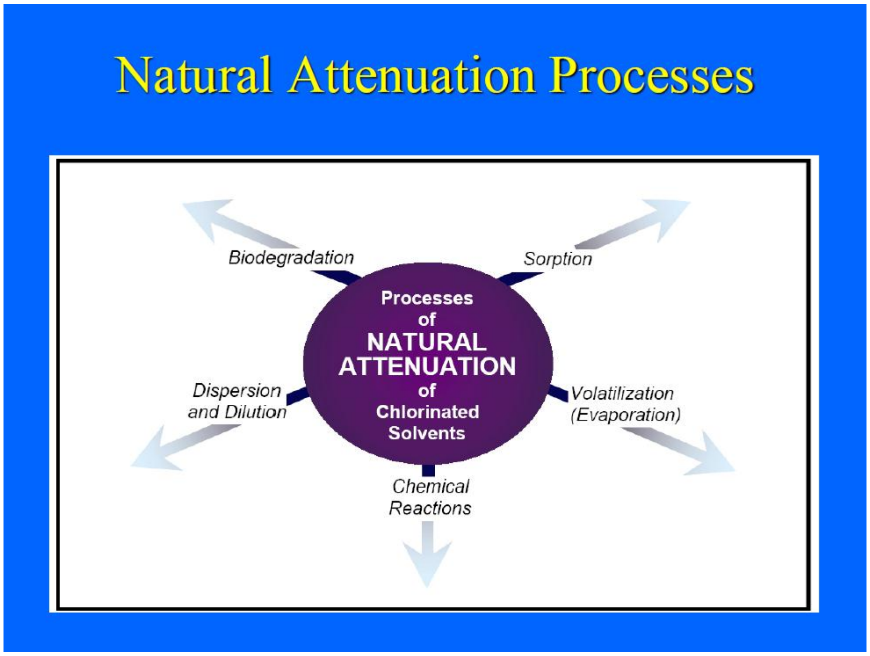
When estimating the extent of LNAPL contamination for remediation, all four phases must be accounted for. For example, if remediation of the dissolved LNAPL is undertaken without considering the adsorbed phase, adsorbed LNAPL chemicals will desorb into the groundwater and keep dissolved concentrations high. Free LNAPL in the formation pores will continue to dissolve into groundwater so that concentrations of dissolved LNAPL will not decrease during remediation.



Dense Non-Aqueous Phase Liquids (DNAPL)

EPA/600/F-98/022 (1999)

Dense non-aqueous phase liquids (DNAPL) have densities greater than water (i.e., specific gravity greater than 1.00) and therefore sink through the water table until a low-permeability material is encountered to stop the vertical downward migration of DNAPL, or the source of DNAPL for vertical downward migration is depleted. Examples of DNAPL are chlorinated solvents (PCE, TCE), creosote, and coal tar. DNAPLs are also soluble in water to some degree. Released DNAPLs penetrate the water table and plumes of dissolved DNAPL move downgradient of the zone of DNAPL pool. In geologic materials DNAPL chemicals also exist in four phases and when estimating the extent of DNAPL contamination for remediation all four phases must be accounted for. Free phase DNAPL does not move in the direction of hydraulic gradient; the plume of dissolved DNAPL chemicals moves downgradient but DNAPL does not move downgradient. DNAPL moves under the influence of gravity *(i.e.*, downward) and will continue to move downward as long as there are pathways to move through and enough DNAPL to "feed" the movement.

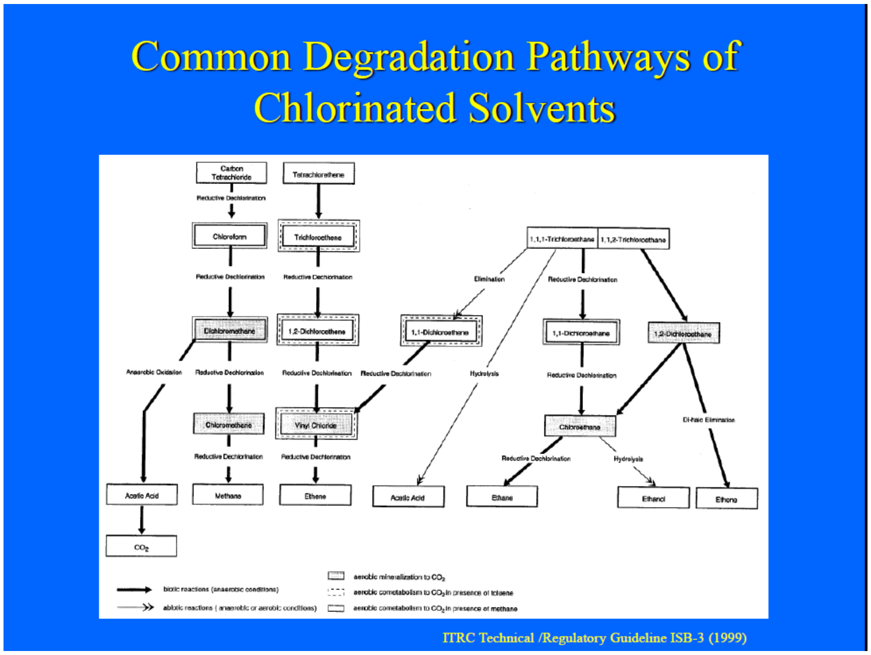


Natural Attenuation Processes

There are several mechanisms for natural attenuation:

- Volatization to pore air
- Sorption to the aquifer matrix
- Mechanical dispersion
- Chemical reactions that immobilize or “deactivate” some chemicals (particularly inorganic chemicals)
- Biodegradation of organic chemicals

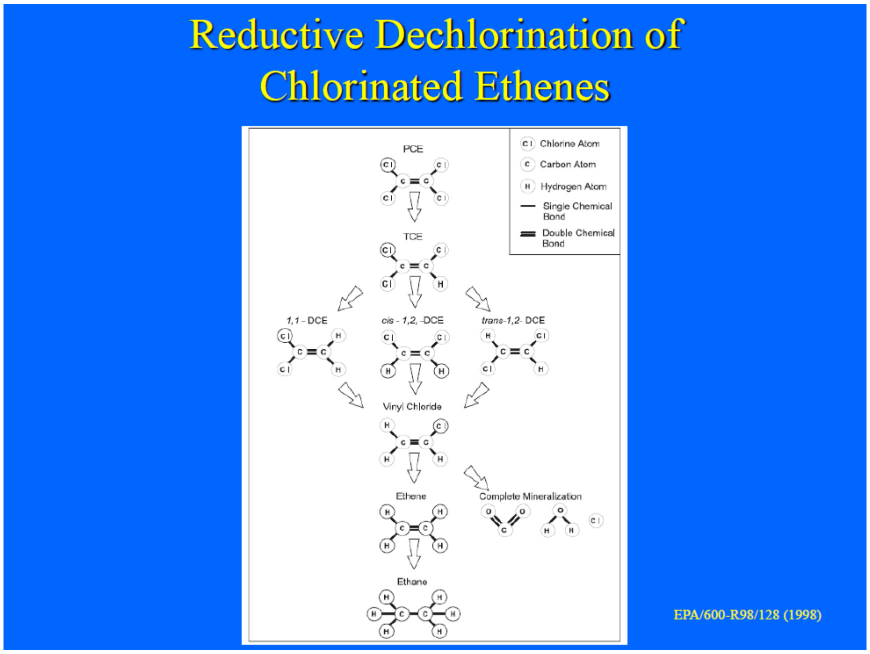
Volatization, sorption, and mechanical dispersion are non-destructive attenuation mechanisms while chemical reactions and biodegradation are usually destructive attenuation mechanisms.



Common Degradation Pathways of Chlorinated Solvents

ITRC Technical /Regulatory Guideline ISB-3 (1999)

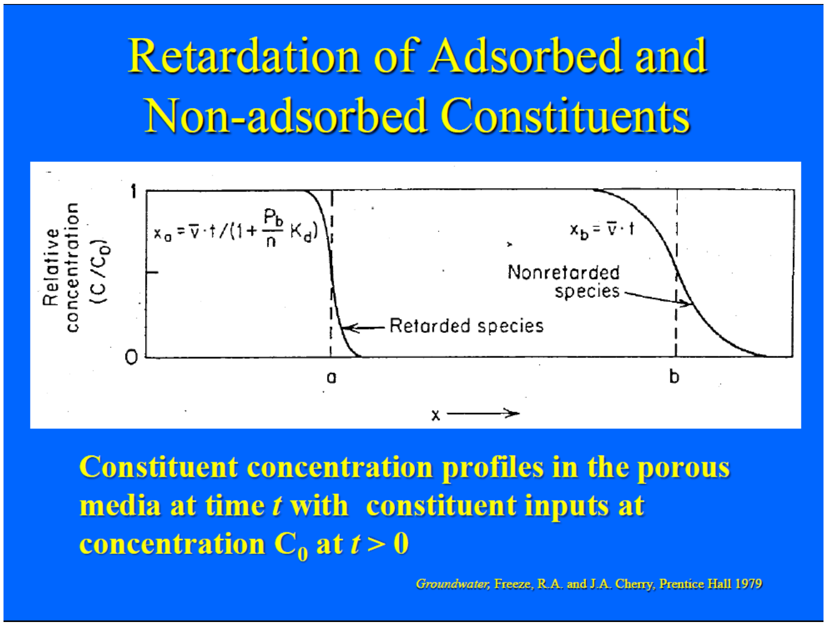
Organic chemicals such as chlorinated ethenes and ethanes degrade to other chemicals. Ethenes have two carbons with a double bond between the carbon atoms (C=C) while ethanes have two carbons with a single bond between the carbon atoms (C-C).



Reductive Dechlorination of Chlorinated Ethenes

EPA/600-R98/128 (1998)

In "reductive" dechlorination reductive refers to the reduction of the number of chlorine atoms (as described previously) and the reduction of the oxidation state of the carbon atoms. Each carbon atom must have four "connections" and each molecule must be electronically neutral. In tetrachloroethene there are two carbon atoms and four chlorine atoms. The oxidation states of the chlorine atoms are "-1" so that the four chlorine atoms equals an electronic charge of –4. Therefore each of the two carbon atoms must have a charge of +2 to make the molecule electronically neutral. In trichloroethene there are two carbon atoms, three chlorine atoms, and one hydrogen atom. The oxidation states of the hydrogen atoms are +1, so one hydrogen atom "neutralizes" the charge on one chlorine atom leaving two chlorine atoms with an electronic charge of –2. Therefore each of the two carbon atoms must have a charge of +1, a reduction in oxidation state from +2 to +1. In dichloroethene there are two carbon atoms, two chlorine atoms, and two hydrogen atoms. The two chlorine atoms (-2) neutralize the electronic charge of the two hydrogen atoms (+2) so that the two carbon atoms have a charge of 0, again reducing the oxidation state. In vinyl chloride there are two carbon atoms, one chlorine atom (-1), and three hydrogen atoms (+3) so that the two carbon atoms have a charge of –1. In ethene there are two carbon atoms and four hydrogen atoms (+4) so that the two carbon atoms have a charge of –2 and in ethane there are two carbon atoms and six hydrogen atoms (+6) so that the two carbon atoms have a charge of –3. The most reduced state of carbon is methane, CH_4, where the single carbon atom must have a charge of –4 to neutralize the +4 charge of the four hydrogen atoms.

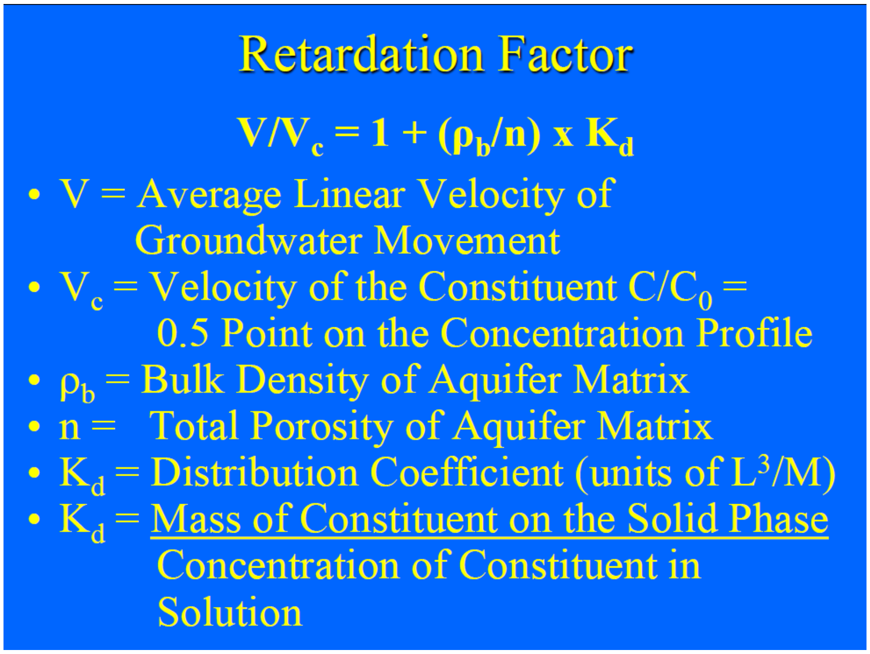


Retardation of Adsorbed and Non-adsorbed Constituents

Constituent concentration profiles in the porous media at time *t* with constituent inputs at concentration C_0 at $t > 0$

Groundwater, Freeze, R.A. and J.A. Cherry, Prentice Hall 1979

Some dissolved constituents react with the aquifer matrix so that movement of the constituents is retarded relative to the movement of groundwater. The concentration profile, caused by dispersion, of a retarded constituent will lag behind the concentration profile of a non-retarded constituent.

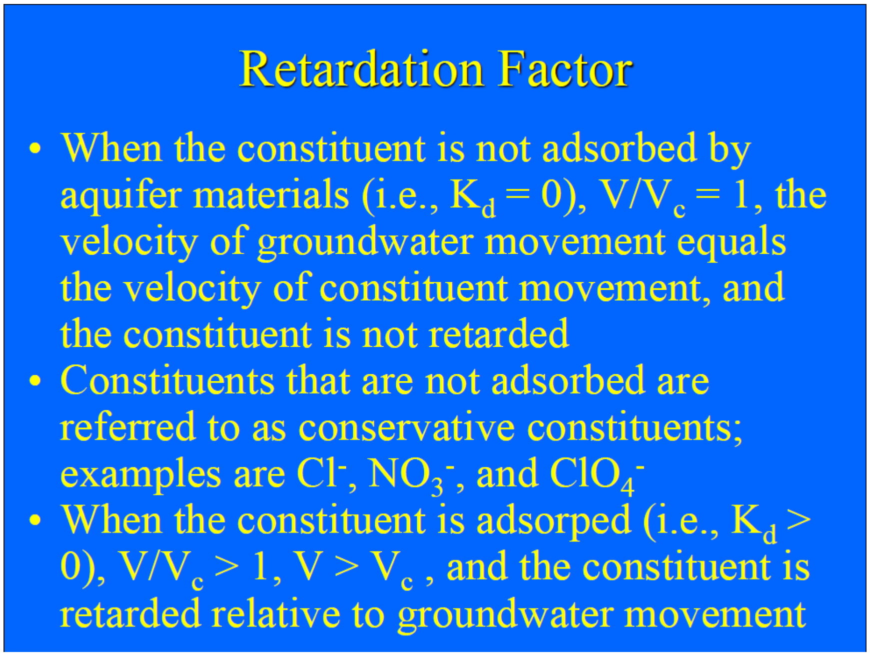


Retardation Factor

$$V/V_c = 1 + (\rho_b/n) \times K_d$$

- V = Average Linear Velocity of Groundwater Movement
- V_c = Velocity of the Constituent C/C_0 = 0.5 Point on the Concentration Profile
- ρ_b = Bulk Density of Aquifer Matrix
- n = Total Porosity of Aquifer Matrix
- K_d = Distribution Coefficient (units of L^3/M)
- $K_d = \dfrac{\text{Mass of Constituent on the Solid Phase}}{\text{Concentration of Constituent in Solution}}$

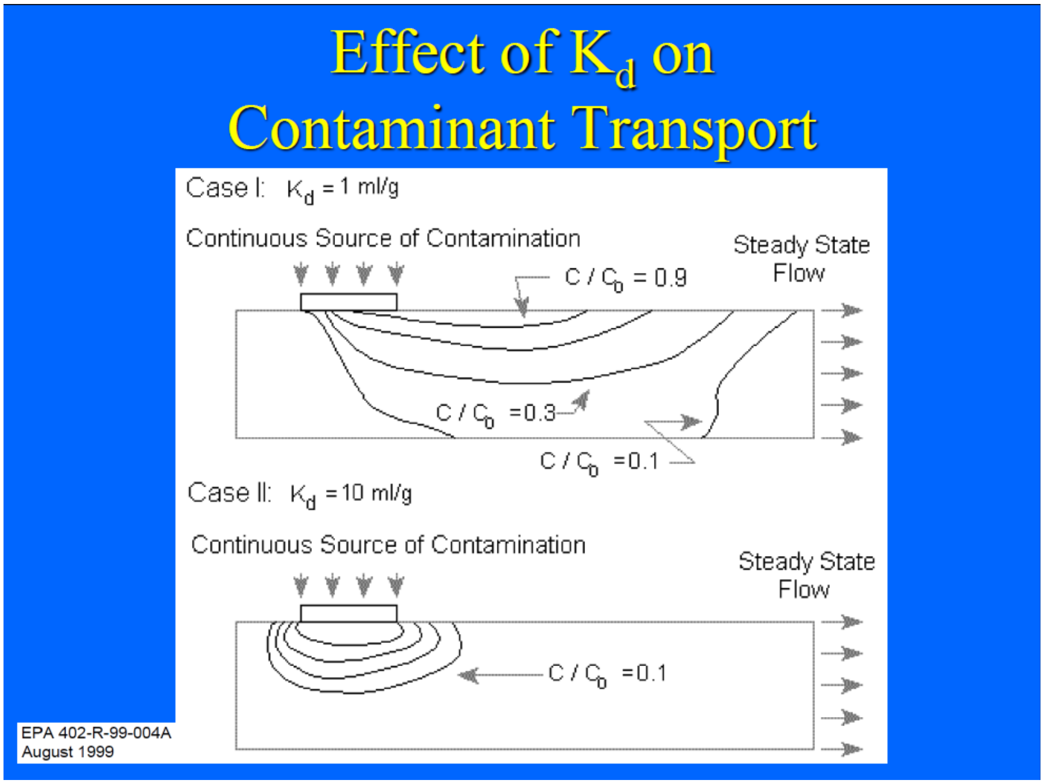
Mathematics of the retardation factor: Variables include bulk density of the aquifer matrix, total (not effective) porosity of the aquifer matrix, and the distribution coefficient which is the ratio between the mass of constituent on the solid matrix of the aquifer and the concentration of the constituent in groundwater. The larger the distribution coefficient the more constituent there is on the aquifer matrix relative to the groundwater concentration.



Retardation Factor

- When the constituent is not adsorbed by aquifer materials (i.e., $K_d = 0$), $V/V_c = 1$, the velocity of groundwater movement equals the velocity of constituent movement, and the constituent is not retarded
- Constituents that are not adsorbed are referred to as conservative constituents; examples are Cl^-, NO_3^-, and ClO_4^-
- When the constituent is adsorped (i.e., $K_d > 0$), $V/V_c > 1$, $V > V_c$, and the constituent is retarded relative to groundwater movement

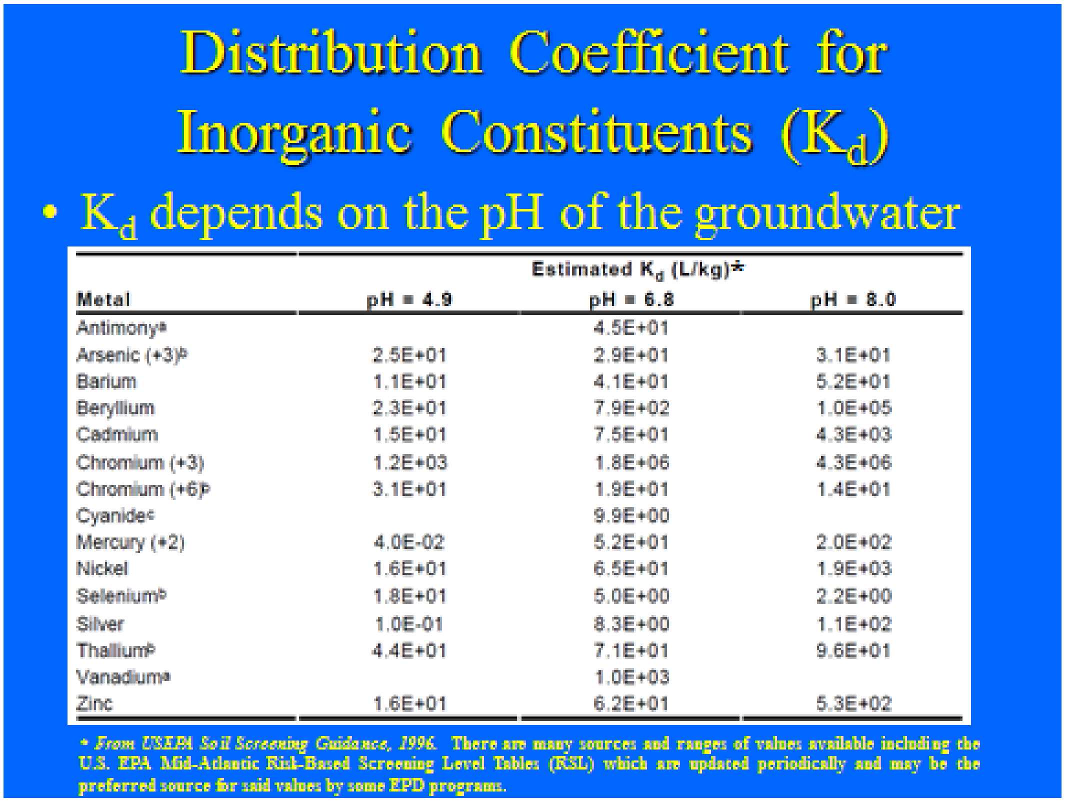
The retardation factor is 1 for conservative constituents that are not adsorbed on the aquifer matrix, have a distribution coefficient of zero, and are therefore not retarded. Conservative constituents that don't react with the aquifer matrix include chloride, nitrate, and perchlorate. For constituents that react with the aquifer matrix and are adsorbed, the distribution coefficient is larger than zero, the retardation factor is greater than one, and the dissolved constituent moves more slowly than the average linear velocity of groundwater movement.



Effect of K_d on Contaminant Transport

EPA 402-R-99-004A
August 1999

Illustration of how distribution coefficient and retardation affects movement of dissolved constituents in groundwater. With a smaller distribution coefficient plumes move further in a given time than with a larger distribution coefficient



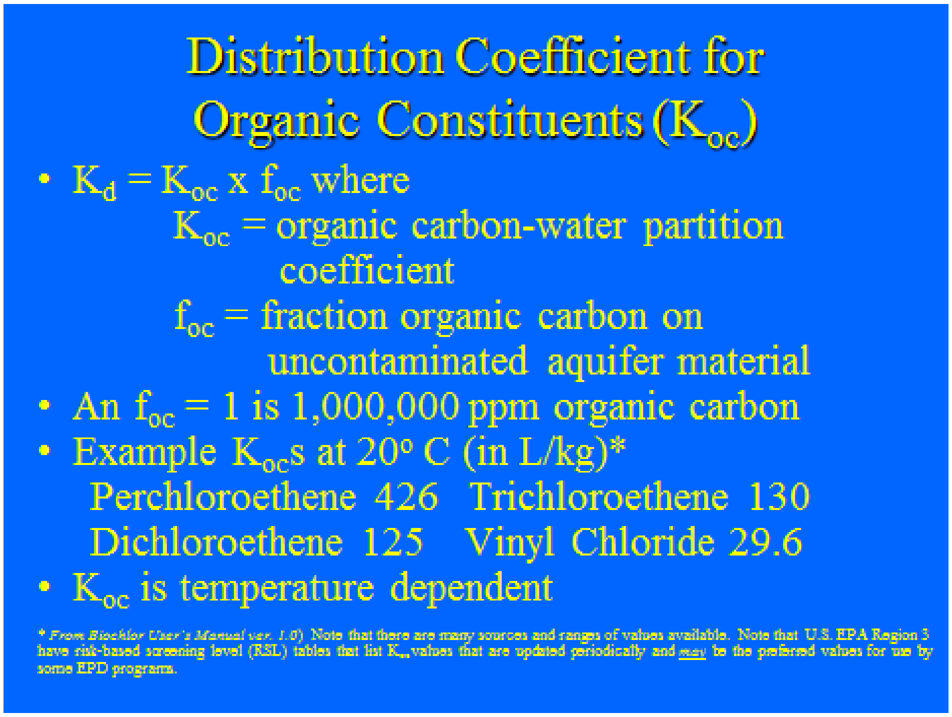
Distribution Coefficient for Inorganic Constituents (K_d)

- K_d depends on the pH of the groundwater

	Estimated K_d (L/kg)*		
Metal	**pH = 4.9**	**pH = 6.8**	**pH = 8.0**
Antimony[a]		4.5E+01	
Arsenic (+3)[b]	2.5E+01	2.9E+01	3.1E+01
Barium	1.1E+01	4.1E+01	5.2E+01
Beryllium	2.3E+01	7.9E+02	1.0E+05
Cadmium	1.5E+01	7.5E+01	4.3E+03
Chromium (+3)	1.2E+03	1.8E+06	4.3E+06
Chromium (+6)[b]	3.1E+01	1.9E+01	1.4E+01
Cyanide[c]		9.9E+00	
Mercury (+2)	4.0E-02	5.2E+01	2.0E+02
Nickel	1.6E+01	6.5E+01	1.9E+03
Selenium[b]	1.8E+01	5.0E+00	2.2E+00
Silver	1.0E-01	8.3E+00	1.1E+02
Thallium[b]	4.4E+01	7.1E+01	9.6E+01
Vanadium[a]		1.0E+03	
Zinc	1.6E+01	6.2E+01	5.3E+02

* *From USEPA Soil Screening Guidance, 1996.* There are many sources and ranges of values available including the U.S. EPA Mid-Atlantic Risk-Based Screening Level Tables (RSL) which are updated periodically and may be the preferred source for said values by some EPD programs.

Distribution coefficients of inorganic constituents depend on the pH of the groundwater. Higher pH (less acidity) does not always mean a larger distribution coefficient (look at hexavalent chromium and selenium).



Distribution Coefficient for Organic Constituents (K_{oc})

- $K_d = K_{oc} \times f_{oc}$ where
  - K_{oc} = organic carbon-water partition coefficient
  - f_{oc} = fraction organic carbon on uncontaminated aquifer material
- An $f_{oc} = 1$ is 1,000,000 ppm organic carbon
- Example K_{oc}s at 20° C (in L/kg)*

Perchloroethene	426	Trichloroethene	130
Dichloroethene	125	Vinyl Chloride	29.6

- K_{oc} is temperature dependent

* *From Biochlor User's Manual ver. 1.0*) Note that there are many sources and ranges of values available. Note that U.S. EPA Region 3 have risk-based screening level (RSL) tables that list K_{oc} values that are updated periodically and may be the preferred values for use by some EPD programs.

Distribution coefficients of organic constituents are equal to the organic carbon-water partition coefficient, a property of the constituent, times the fraction of organic carbon in the uncontaminated aquifer matrix (i.e., the amount of organic carbon available to adsorb the organic constituent). Fraction organic carbon is different than concentration of total organic carbon (TOC). A fraction organic carbon of 1 is a TOC concentration of 1,000,000 ppm, a fraction organic carbon of 0.1 is a TOC concentration of 100,000 ppm, and a fraction organic carbon of 0.01 is a TOC concentration of 10,000 ppm. Organic carbon-water partition coefficient is temperature dependent, particularly for volatile organic compounds

First Order Decay

- First Order Decay Equation

$$C_2 = C_1 e^{-\lambda \Delta t}$$

- First Order Decay Coefficient

$$\lambda = (\ln C_1 - \ln C_2)/\Delta t = 0.693/t_{1/2}$$

- Half Lives (years)

Perchloroethene	0.58 – 9.9	Trichloroethene	0.77 – 13.9
Dichloroethene	0.21 - 3.9	Vinyl Chloride	0.27 – 5.8

- First Order Decay Coefficients (units of 1/yr)

Perchloroethene	0.07 - 1.20	Trichloroethene	0.05 - 0.9
Dichloroethene	0.18 - 3.3	Vinyl Chloride	0.12 - 2.6

Constituents can decay be first order decay. The first order decay equation is exponential with time in the exponent. The first order decay coefficient is related to the half-life of the dissolved constituent. While the retardation factor equation is linear, the first order decay equation is exponential. A larger retardation factor allows more half lives for contaminant attenuation. If an initial concentration is 600µg/L, the travel time to a target is 5 years, and the half life is 1 year, the concentration at the target would be 600 µg/L x 0.5 x 0.5 x 0.5 x 0.5 x 0.5 = 18.75 µg/L. This would be above an MCL of 5 µg/L. If the retardation was twice as large, the travel time to the target would be 10 years and the concentration at the target would be 600 µg/Lx 0.5 x 0.5 x 0.5 x 0.5 x 0.5 x 0.5 x 0.5 x 0.5 x 0.5 x 0.5 = 0.59 µg/L. This would be below an MCL of 5 µg/L. In this example a factor of 2 in the retardation factor resulted in a factor of about 32 in the constituent concentration at the target. This is why getting retardation correct in an assessment is important

Sensitivity of K_d of Organic Constituents to f_{oc}

- Fate and transport models are typically very sensitive to input values of fraction organic carbon used to calculate retardation factors for organic contaminants
- Sensitivity to foc in a BIOCHLOR fate and transport model for chlorinated ethenes

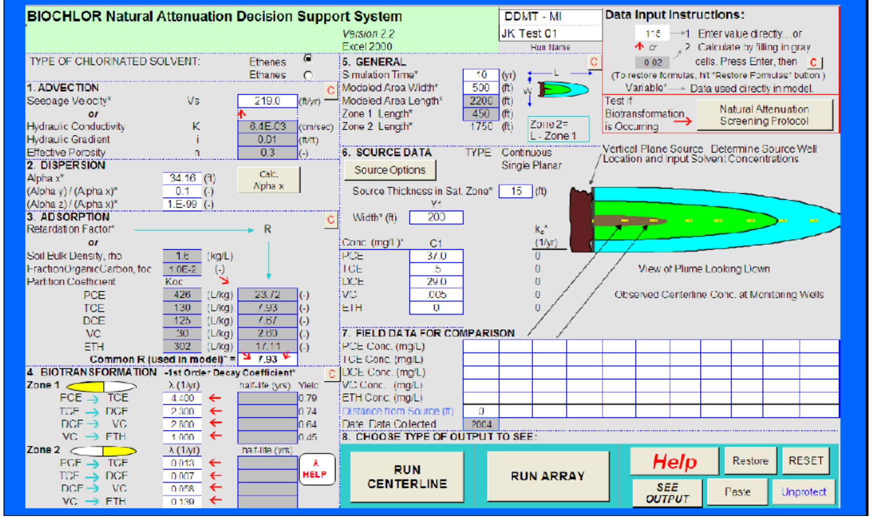
  $f_{oc} = 0.01$ (10,000 ppm)

  $f_{oc} = 0.001$ (1,000 ppm)

Fate and transport models of organic constituents are very sensitive to the fraction organic carbon used in the calculations.

Examples: Sensitivity of Biochlor to f_{oc} Values

BIOCHLOR Model Setup for $f_{oc} = 0.01$ (10,000 ppm)



BIOCHLOR Natural Attenuation Decision Support System
Version 2.2
Excel 2000

DDMT - MI
JK Test 01
Run Name

TYPE OF CHLORINATED SOLVENT: Ethenes ● Ethanes ○

1. ADVECTION
Seepage Velocity* Vs 219.0 (ft/yr)
or
Hydraulic Conductivity K 6.4E-03 (cm/sec)
Hydraulic Gradient i 0.01 (ft/ft)
Effective Porosity n 0.3 (-)

2. DISPERSION
Alpha x* 34.16 (ft)
(Alpha y) / (Alpha x)* 0.1 (-)
(Alpha z) / (Alpha x)* 1.E-99 (-)

3. ADSORPTION
Retardation Factor* R
or
Soil Bulk Density, rho 1.6 (kg/L)
FractionOrganicCarbon, foc 1.0E-2 (-)
Partition Coefficient Koc

	Koc		R	
PCE	426	(L/kg)	23.72	(-)
TCE	130	(L/kg)	7.93	(-)
DCE	125	(L/kg)	7.67	(-)
VC	30	(L/kg)	2.60	(-)
ETH	302	(L/kg)	17.11	(-)

Common R (used in model)* = 7.93

4. BIOTRANSFORMATION -1st Order Decay Coefficient*

Zone 1	λ (1/yr)	half-life (yrs)	Yield
PCE → TCE	4.400		0.79
TCE → DCE	2.300		0.74
DCE → VC	2.800		0.64
VC → ETH	1.000		0.45

Zone 2	λ (1/yr)	half-life (yrs)
PCE → TCE	0.013	
TCE → DCE	0.007	
DCE → VC	0.058	
VC → ETH	0.139	

5. GENERAL
Simulation Time* 10 (yr)
Modeled Area Width* 500 (ft)
Modeled Area Length* 2200 (ft)
Zone 1 Length* 450 (ft)
Zone 2 Length* 1750 (ft)
Zone 2= L - Zone 1

Data Input Instructions:
1. Enter value directly....or
2. Calculate by filling in gray cells. Press Enter, then C
(To restore formulas, hit "Restore Formulas" button)
Variable* → Data used directly in model.
Test if Biotransformation is Occurring

6. SOURCE DATA TYPE: Continuous Single Planar
Vertical Plane Source: Determine Source Well Location and Input Solvent Concentrations
Source Thickness in Sat. Zone* 15 (ft)
Width* (ft) Y1 200

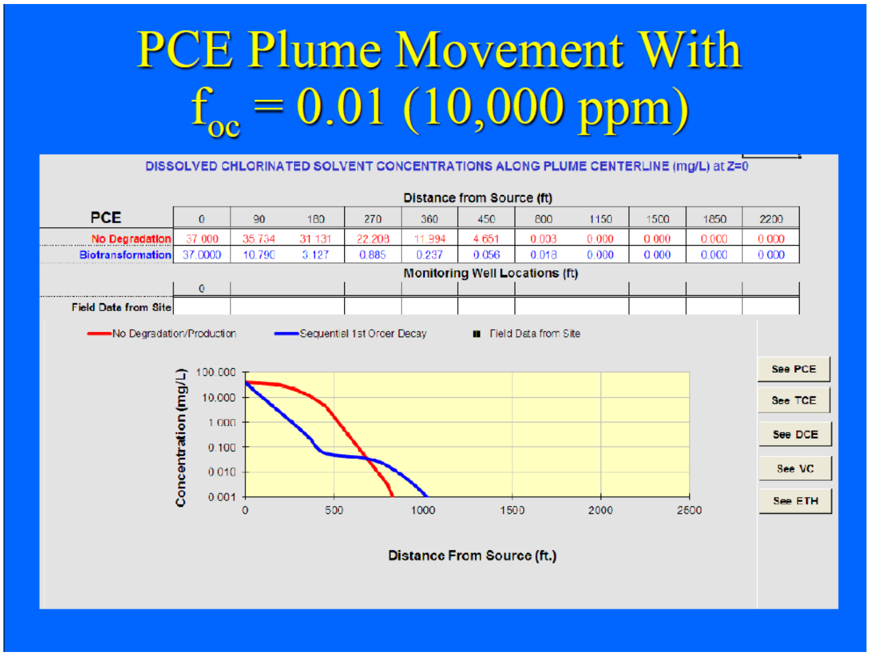
Conc. (mg/L)*	C1	k_s* (1/yr)
PCE	37.0	0
TCE	.5	0
DCE	29.0	0
VC	.005	0
ETH	0	0

View of Plume Looking Down
Observed Centerline Conc. at Monitoring Wells

7. FIELD DATA FOR COMPARISON
PCE Conc. (mg/L)
TCE Conc. (mg/L)
DCE Conc. (mg/L)
VC Conc. (mg/L)
ETH Conc. (mg/L)
Distance from Source (ft) 0
Date Data Collected 2004

8. CHOOSE TYPE OF OUTPUT TO SEE:

BIOCHLOR model for fate and transport of chlorinated ethenes set up with a fraction organic carbon of 0.01 (10,000 ppm TOC).



PCE Plume Movement With $f_{oc} = 0.01$ (10,000 ppm)

DISSOLVED CHLORINATED SOLVENT CONCENTRATIONS ALONG PLUME CENTERLINE (mg/L) at Z=0

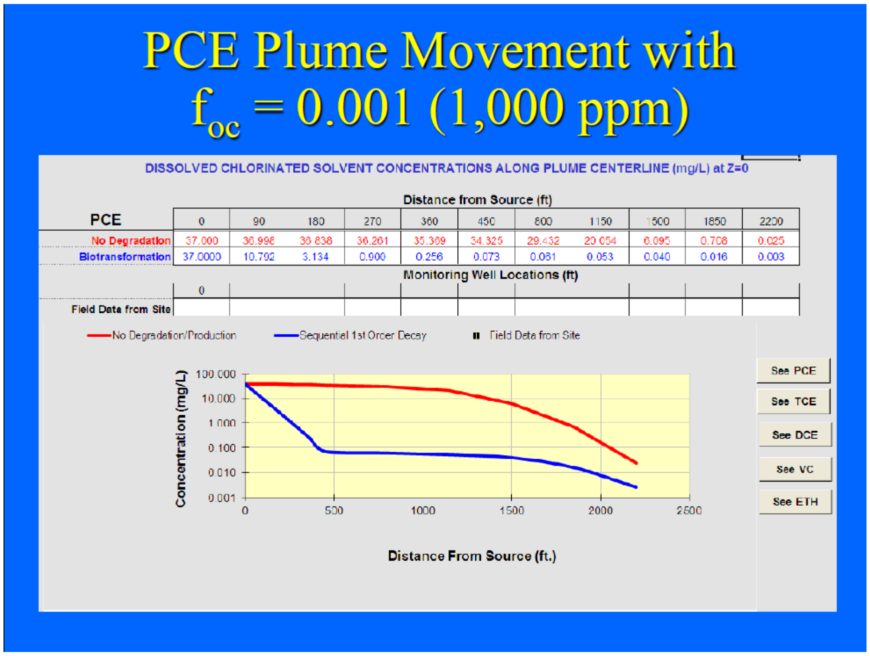
Distance from Source (ft)

PCE	0	90	180	270	360	450	800	1150	1500	1850	2200
No Degradation	37.000	35.734	31.131	22.208	11.994	4.651	0.003	0.000	0.000	0.000	0.000
Biotransformation	37.0000	10.790	3.127	0.885	0.237	0.056	0.018	0.000	0.000	0.000	0.000

Monitoring Well Locations (ft)

	0									
Field Data from Site										

With a fraction organic carbon of 0.01 the model predicts that detectable PCE will travel less than 1,150 feet from the source.



PCE Plume Movement with $f_{oc} = 0.001$ (1,000 ppm)

DISSOLVED CHLORINATED SOLVENT CONCENTRATIONS ALONG PLUME CENTERLINE (mg/L) at Z=0

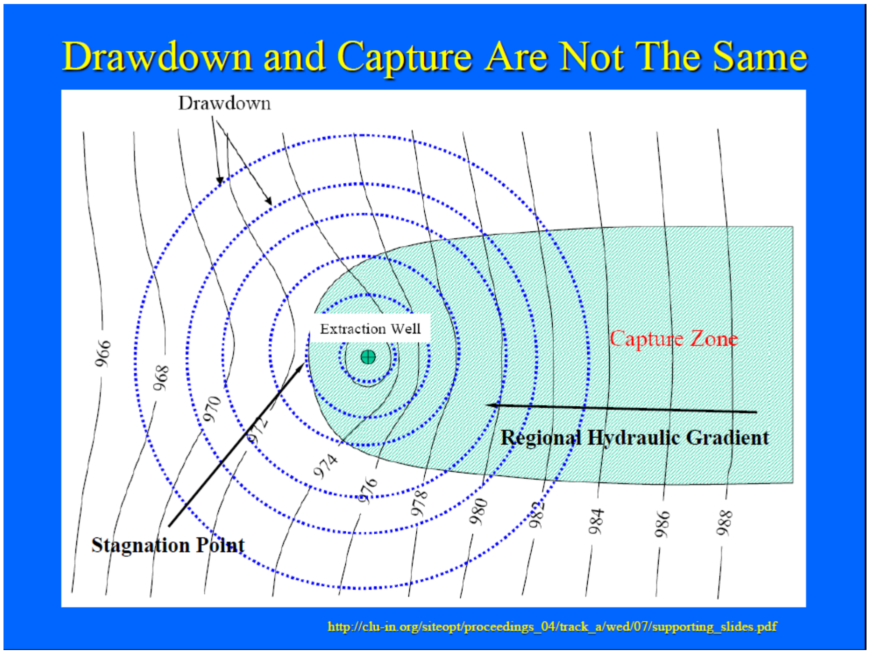
Distance from Source (ft)

PCE	0	90	180	270	360	450	800	1150	1500	1850	2200
No Degradation	37.000	36.998	36.838	36.261	35.369	34.325	29.432	20.054	6.095	0.708	0.025
Biotransformation	37.0000	10.792	3.134	0.900	0.256	0.073	0.061	0.053	0.040	0.016	0.003

Monitoring Well Locations (ft)

	0									
Field Data from Site										

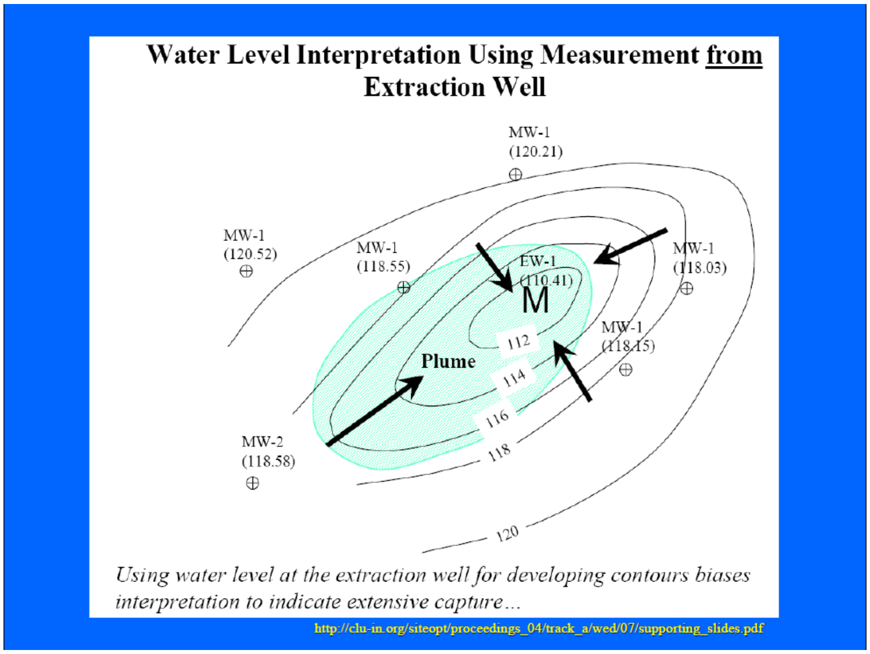
With a fraction organic carbon of 0.001 the model predicts detectable PCE will travel more than 2,200 feet from the source.



Drawdown and Capture Are Not The Same

http://clu-in.org/siteopt/proceedings_04/track_a/wed/07/supporting_slides.pdf

An extraction well will create a cone-of-depression where water levels are drawn down. The cone-of-depression is <u>not</u> the same as the capture zone of the extraction well. The cone-of-depression must be superimposed on the regional groundwater flow field to determine the capture zone. The well capture zone will extend up the regional hydraulic gradient beyond the cone-of-depression. The capture zone will extend downgradient to the stagnation point where groundwater is no longer is captured by the extraction well. The stagnation point is within the downgradient extent of the cone-of-depression. In other words, the capture zone extends further upgradient than the cone-of-depression and does not extend as far downgradient as the cone-of-depression.

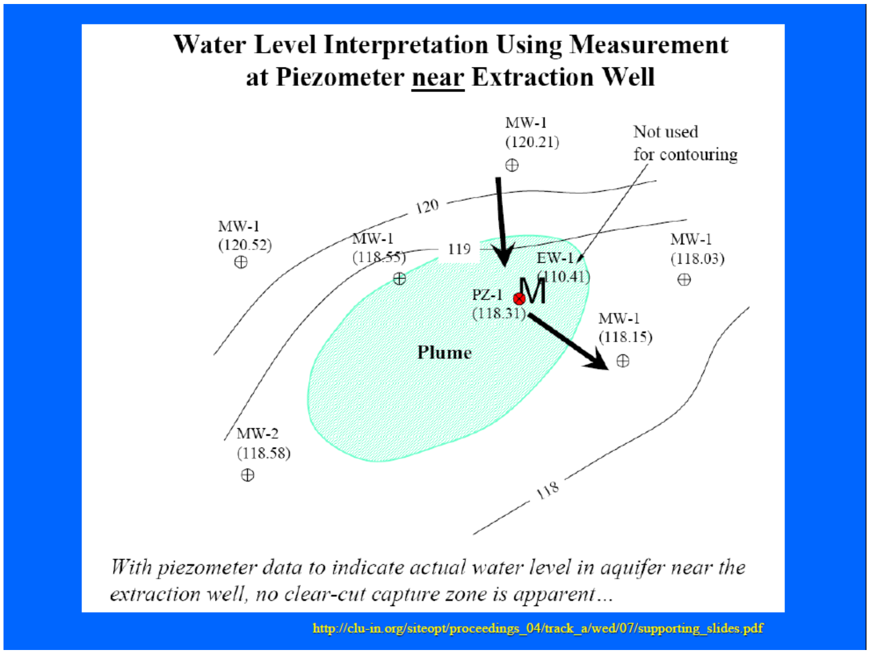


Water Level Interpretation Using Measurement <u>from</u> Extraction Well

Using water level at the extraction well for developing contours biases interpretation to indicate extensive capture…

http://clu-in.org/siteopt/proceedings_04/track_a/wed/07/supporting_slides.pdf

When determining capture zones of extraction wells, hydraulic heads in extraction wells should not be used to draw potentiometric surface contours or determine directions of groundwater movement. Water levels in extraction wells are lower than in the aquifer around the extraction well due to friction head-losses as groundwater enters the wells. The hydraulic head at well EW-1 (110.41 feet) is lower than the hydraulic head of the aquifer around well EW-1, and including the water level at EW-1 in the potentiometric surface map, over-estimates the extraction well capture zone.



Water Level Interpretation Using Measurement at Piezometer near Extraction Well

With piezometer data to indicate actual water level in aquifer near the extraction well, no clear-cut capture zone is apparent…

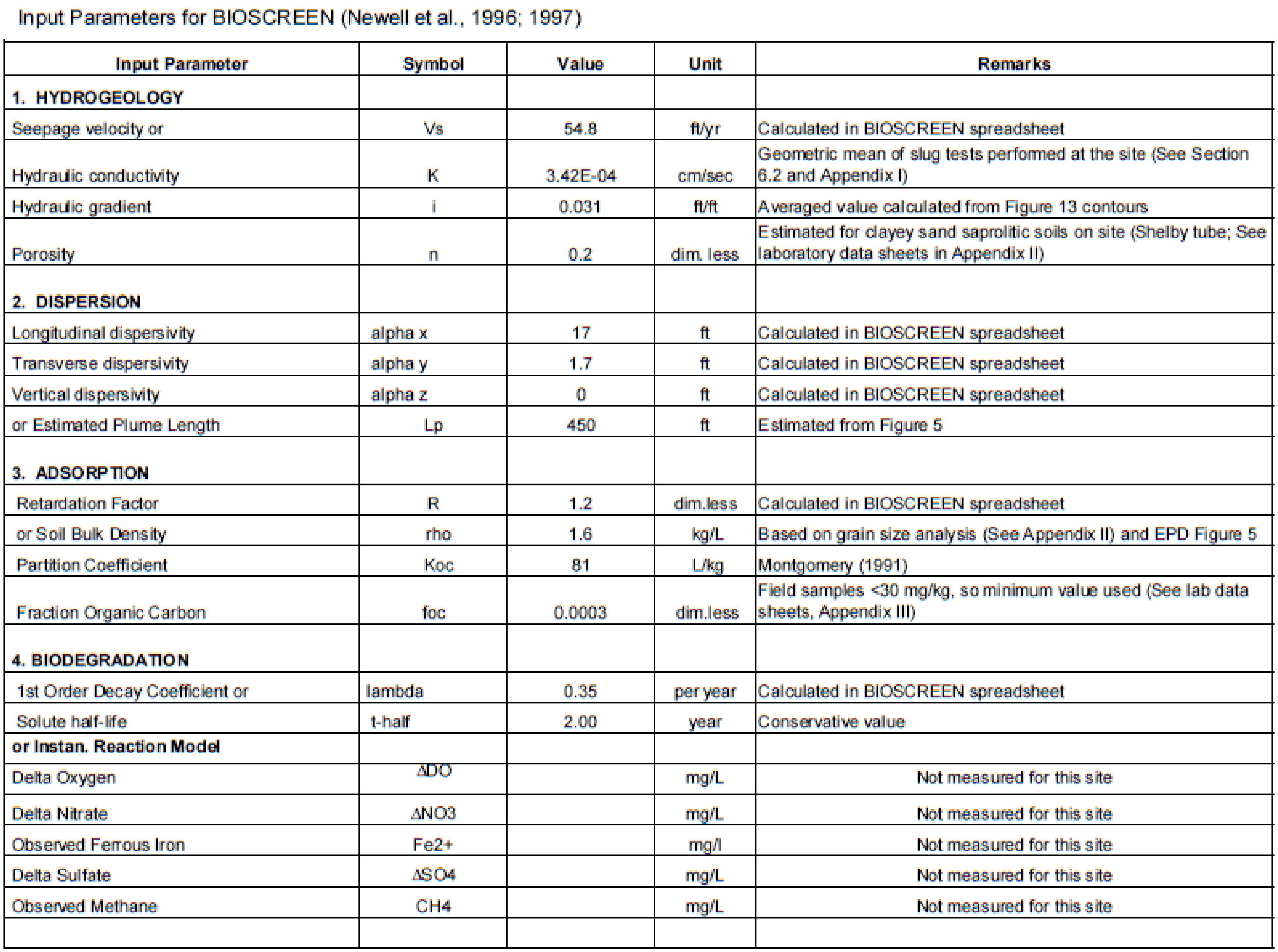
http://clu-in.org/siteopt/proceedings_04/track_a/wed/07/supporting_slides.pdf

A piezometer near well EW-1 indicated a hydraulic head of 118.31 feet, much higher than the hydraulic head in the extraction well. The potentiometric surface map properly drawn using the hydraulic head at the piezometer rather than the extraction well depicts a much different (in fact nonexistent) extraction well capture zone.

APPENDIX B: Example Data Input Spreadsheets

Example Data Summary Sheet for BIOSCREEN Model

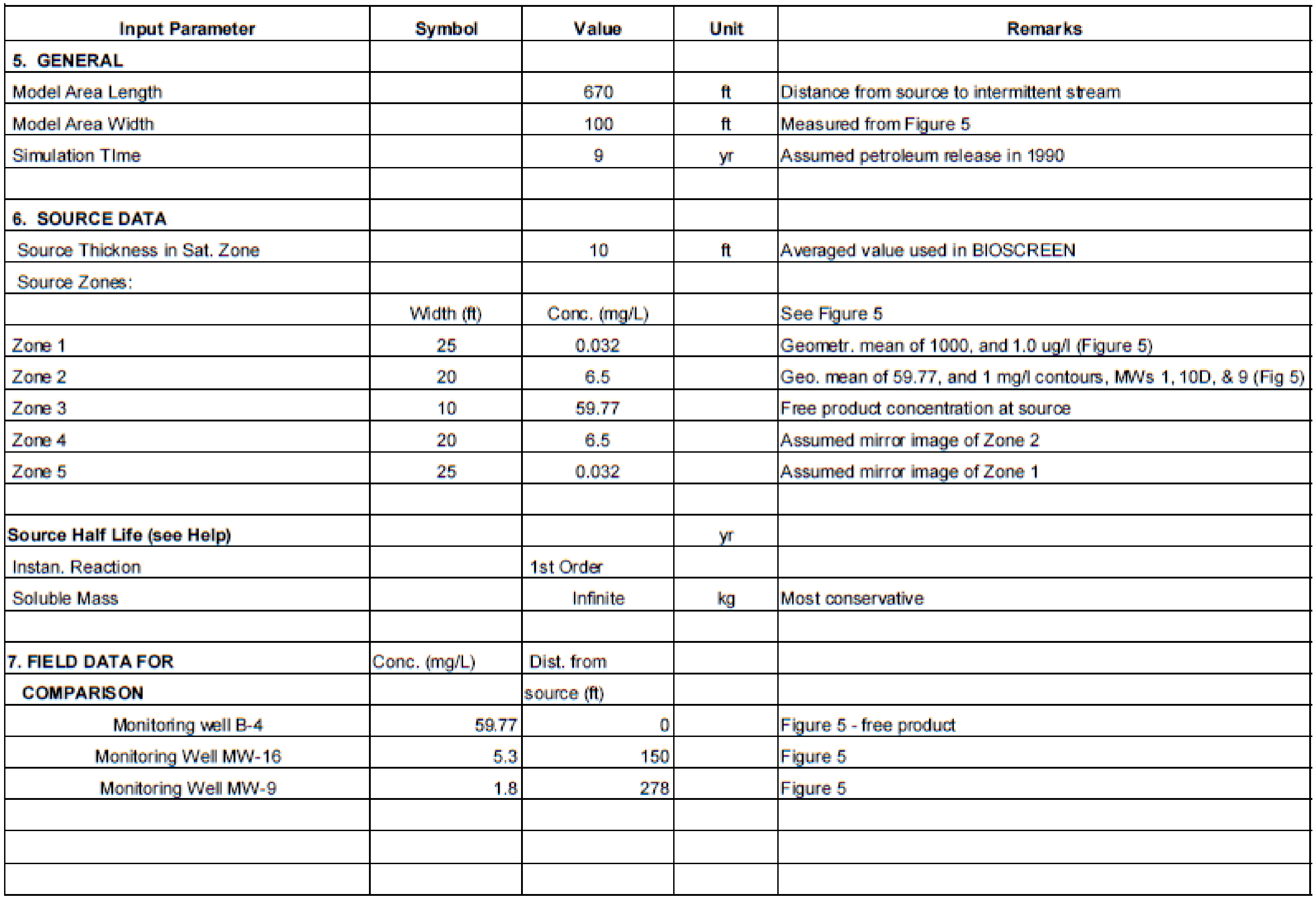
(from Introduction to Fate and Groundwater Modeling Seminar, 1999, Georgia Ground Water Association, Doraville, Georgia)



Input Parameters for BIOSCREEN (Newell et al., 1996; 1997)

Input Parameter	Symbol	Value	Unit	Remarks
1. HYDROGEOLOGY				
Seepage velocity or	Vs	54.8	ft/yr	Calculated in BIOSCREEN spreadsheet
Hydraulic conductivity	K	3.42E-04	cm/sec	Geometric mean of slug tests performed at the site (See Section 6.2 and Appendix I)
Hydraulic gradient	i	0.031	ft/ft	Averaged value calculated from Figure 13 contours
Porosity	n	0.2	dim. less	Estimated for clayey sand saprolitic soils on site (Shelby tube; See laboratory data sheets in Appendix II)
2. DISPERSION				
Longitudinal dispersivity	alpha x	17	ft	Calculated in BIOSCREEN spreadsheet
Transverse dispersivity	alpha y	1.7	ft	Calculated in BIOSCREEN spreadsheet
Vertical dispersivity	alpha z	0	ft	Calculated in BIOSCREEN spreadsheet
or Estimated Plume Length	Lp	450	ft	Estimated from Figure 5
3. ADSORPTION				
Retardation Factor	R	1.2	dim.less	Calculated in BIOSCREEN spreadsheet
or Soil Bulk Density	rho	1.6	kg/L	Based on grain size analysis (See Appendix II) and EPD Figure 5
Partition Coefficient	Koc	81	L/kg	Montgomery (1991)
Fraction Organic Carbon	foc	0.0003	dim.less	Field samples <30 mg/kg, so minimum value used (See lab data sheets, Appendix III)
4. BIODEGRADATION				
1st Order Decay Coefficient or	lambda	0.35	per year	Calculated in BIOSCREEN spreadsheet
Solute half-life	t-half	2.00	year	Conservative value
or Instan. Reaction Model				
Delta Oxygen	ΔDO		mg/L	Not measured for this site
Delta Nitrate	ΔNO3		mg/L	Not measured for this site
Observed Ferrous Iron	Fe2+		mg/l	Not measured for this site
Delta Sulfate	ΔSO4		mg/L	Not measured for this site
Observed Methane	CH4		mg/L	Not measured for this site

Input Parameters for BIOSCREEN (Newell et al., 1996; 1997)

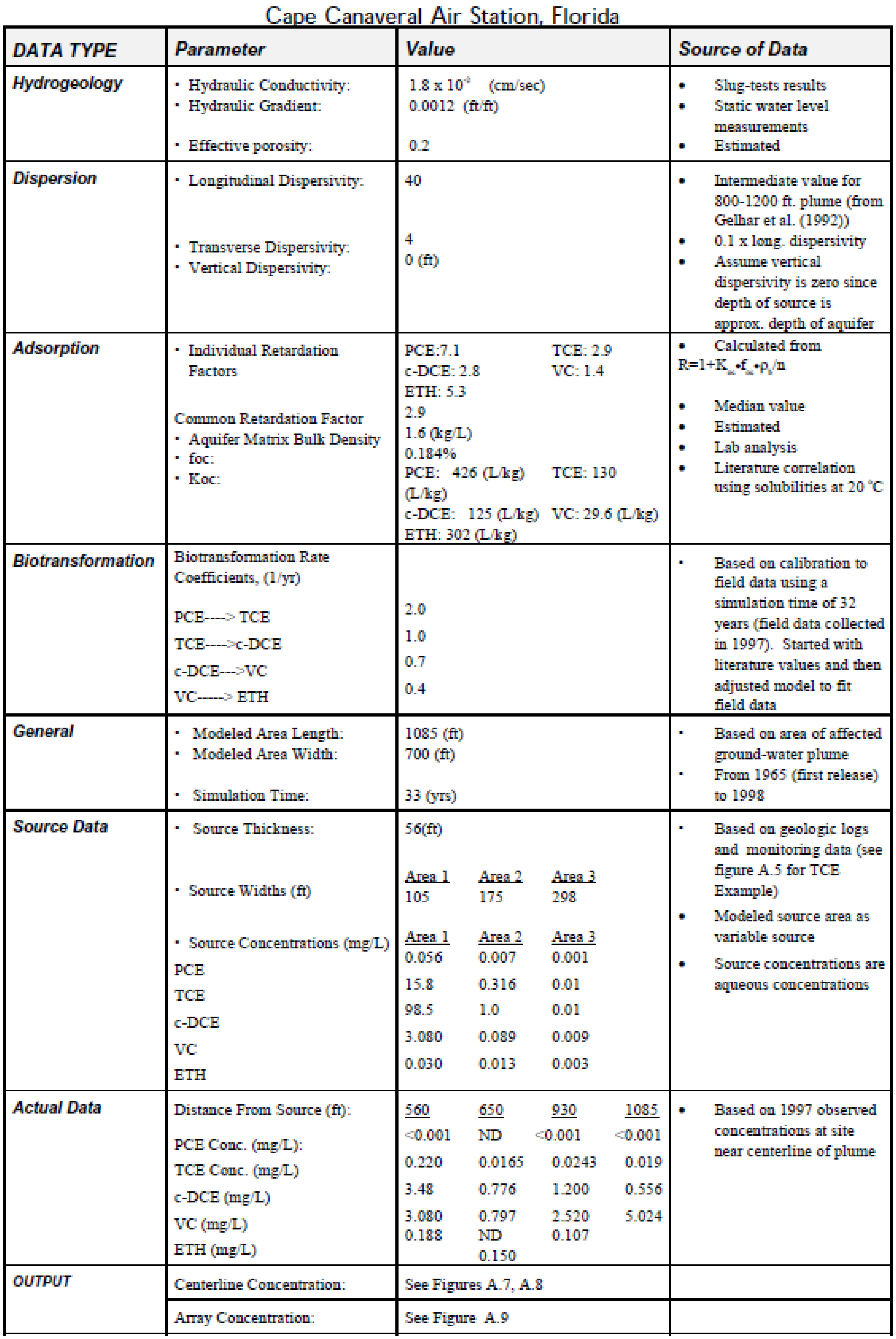


Input Parameter	Symbol	Value	Unit	Remarks
5. GENERAL				
Model Area Length		670	ft	Distance from source to intermittent stream
Model Area Width		100	ft	Measured from Figure 5
Simulation TIme		9	yr	Assumed petroleum release in 1990
6. SOURCE DATA				
Source Thickness in Sat. Zone		10	ft	Averaged value used in BIOSCREEN
Source Zones:				
	Width (ft)	Conc. (mg/L)		See Figure 5
Zone 1	25	0.032		Geometr. mean of 1000, and 1.0 ug/l (Figure 5)
Zone 2	20	6.5		Geo. mean of 59.77, and 1 mg/l contours, MWs 1, 10D, & 9 (Fig 5)
Zone 3	10	59.77		Free product concentration at source
Zone 4	20	6.5		Assumed mirror image of Zone 2
Zone 5	25	0.032		Assumed mirror image of Zone 1
Source Half Life (see Help)			yr	
Instan. Reaction		1st Order		
Soluble Mass		Infinite	kg	Most conservative
7. FIELD DATA FOR	Conc. (mg/L)	Dist. from		
COMPARISON		source (ft)		
Monitoring well B-4	59.77	0		Figure 5 - free product
Monitoring Well MW-16	5.3	150		Figure 5
Monitoring Well MW-9	1.8	278		Figure 5

Note: Input values and remarks shown above are examples only. References to figures do not refer to figures contained within this guidance document. Furthermore, the source of, and justification for, input values used in modeling effort should be included in the "Remarks" column.

Example Data Summary Sheet for BIOCHLOR Model

(from Biochlor Natural Attenuation Decision Support System User's Manual, Version 1.0)



Cape Canaveral Air Station, Florida

DATA TYPE	Parameter	Value	Source of Data
Hydrogeology	▪ Hydraulic Conductivity: ▪ Hydraulic Gradient: ▪ Effective porosity:	1.8×10^{-4} (cm/sec) 0.0012 (ft/ft) 0.2	• Slug-tests results • Static water level measurements • Estimated
Dispersion	▪ Longitudinal Dispersivity: ▪ Transverse Dispersivity: ▪ Vertical Dispersivity:	40 4 0 (ft)	• Intermediate value for 800-1200 ft. plume (from Gelhar et al. (1992)) • 0.1 x long. dispersivity • Assume vertical dispersivity is zero since depth of source is approx. depth of aquifer
Adsorption	▪ Individual Retardation Factors Common Retardation Factor ▪ Aquifer Matrix Bulk Density ▪ foc: ▪ Koc:	PCE:7.1 TCE: 2.9 c-DCE: 2.8 VC: 1.4 ETH: 5.3 2.9 1.6 (kg/L) 0.184% PCE: 426 (L/kg) TCE: 130 (L/kg) c-DCE: 125 (L/kg) VC: 29.6 (L/kg) ETH: 302 (L/kg)	• Calculated from $R=1+K_{oc} \cdot f_{oc} \cdot \rho_b/n$ • Median value • Estimated • Lab analysis • Literature correlation using solubilities at 20 °C
Biotransformation	Biotransformation Rate Coefficients, (1/yr) PCE----> TCE TCE---->c-DCE c-DCE--->VC VC-----> ETH	 2.0 1.0 0.7 0.4	▪ Based on calibration to field data using a simulation time of 32 years (field data collected in 1997). Started with literature values and then adjusted model to fit field data
General	▪ Modeled Area Length: ▪ Modeled Area Width: ▪ Simulation Time:	1085 (ft) 700 (ft) 33 (yrs)	▪ Based on area of affected ground-water plume ▪ From 1965 (first release) to 1998
Source Data	▪ Source Thickness: ▪ Source Widths (ft) ▪ Source Concentrations (mg/L) PCE TCE c-DCE VC ETH	56(ft) <u>Area 1</u> <u>Area 2</u> <u>Area 3</u> 105 175 298 <u>Area 1</u> <u>Area 2</u> <u>Area 3</u> 0.056 0.007 0.001 15.8 0.316 0.01 98.5 1.0 0.01 3.080 0.089 0.009 0.030 0.013 0.003	▪ Based on geologic logs and monitoring data (see figure A.5 for TCE Example) • Modeled source area as variable source • Source concentrations are aqueous concentrations
Actual Data	Distance From Source (ft): PCE Conc. (mg/L): TCE Conc. (mg/L) c-DCE (mg/L) VC (mg/L) ETH (mg/L)	<u>560</u> <u>650</u> <u>930</u> <u>1085</u> <0.001 ND <0.001 <0.001 0.220 0.0165 0.0243 0.019 3.48 0.776 1.200 0.556 3.080 0.797 2.520 5.024 0.188 ND 0.107 0.150	• Based on 1997 observed concentrations at site near centerline of plume
OUTPUT	Centerline Concentration:	See Figures A.7, A.8	
	Array Concentration:	See Figure A.9	

Note: Input values and remarks shown are examples only. References to figures do not refer to figures contained within this guidance document. Furthermore, the source of, and justification for, input values used in your modeling effort should be included in the "Remarks" column.