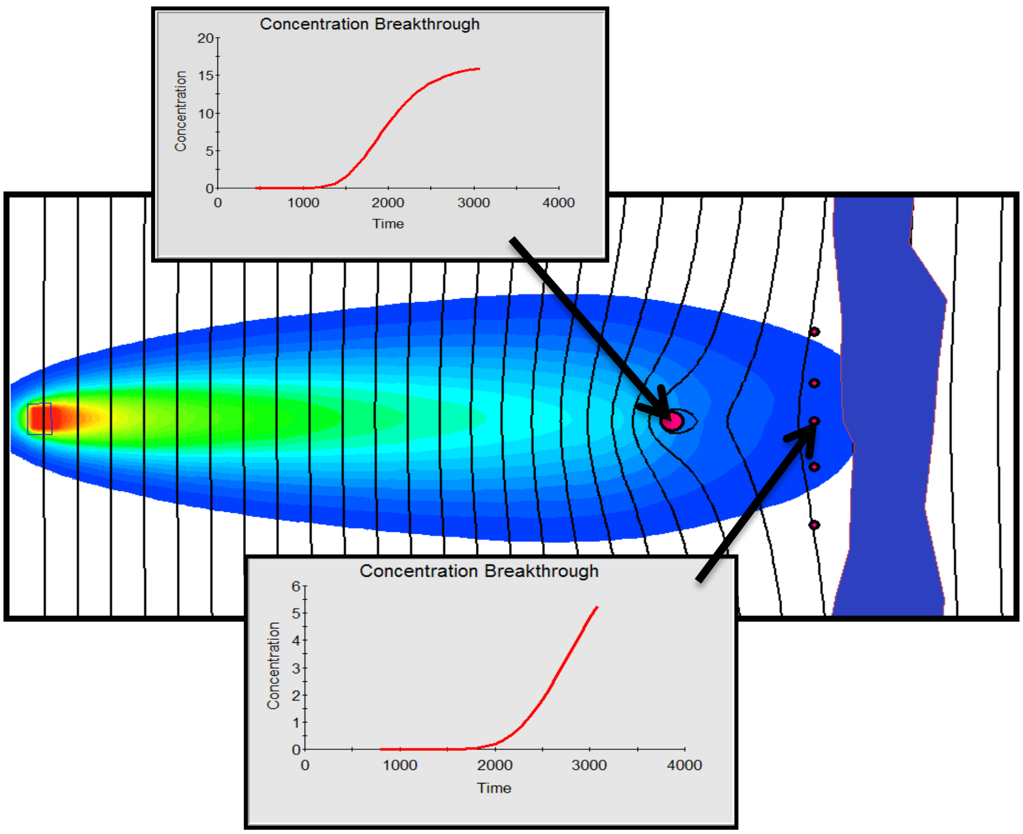
Remediation and
Redevelopment Division

Michigan Department of Environmental Quality

GROUNDWATER MODELING

REMEDIATION AND REDEVELOPMENT DIVISION RESOURCE MATERIALS



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Protecting Michigan's Environment. Ensuring Michigan's Future.

In order to promote a consistent and informed approach for Michigan Department of Environmental Quality (MDEQ) staff, this document was developed to provide information to MDEQ staff and contractors developing or reviewing groundwater models.

This document is available as a technical reference to assist any party in the application and development of groundwater-flow and solute-transport models, and the proper documentation and presentation of simulations for models that have been developed in support of remedial and corrective actions.

This document is explanatory and does not contain any regulatory requirements. It does not establish or affect the legal rights or obligations for groundwater modeling. It does not have the force or effect of law and is not legally binding on the public or the regulated community. Any regulatory decisions made by the MDEQ regarding groundwater modeling will be made by applying the governing statutes and Administrative Rules to relevant facts.

Approved: Robert Wagner

Robert Wagner, Chief
Remediation and Redevelopment Division
February 3, 2014

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SUMMARY

This document is provided to assist environmental professionals in the use of models (numerical and analytical) that are developed in support of remedial decisions at a facility[1] with groundwater contamination. At such facilities, models have been applied to evaluate many aspects of the impact of remedial or corrective actions on groundwater contamination including: determining the effectiveness of hydraulic containment systems, estimating contaminant removal rate and cleanup time, evaluating the potential impact to downgradient receptors such surface water bodies or potable water supply wells, and predicting contaminant concentrations for natural attenuation remedies.

It is important to understand that models are conceptual descriptions, or approximations, that describe physical systems through the use of mathematical equations – they are not exact descriptions of physical systems or processes. The applicability, or usefulness, of a model depends on how closely the mathematical equations approximate the physical system being modeled. For this reason, models that are based on a thorough understanding of the physical system and the assumptions embedded in the derivation of the mathematical equations produce better predictions.

The selection and proper use of a model also relies on a thorough understanding of the importance of relevant flow or solute-transport processes at a facility, which includes proper facility characterization. Proper characterization involves the collection of facility-specific data that accurately describe the movement of groundwater and the disposition of solutes at the facility. However, there is a growing tendency to use values derived from the literature for most model parameters, even those that can be determined by conducting a focused facility investigation. Without proper characterization, and the collection of facility-specific data, it is not possible to determine whether the model equations are appropriate, or even to develop a reasonable model.

Once a facility has been properly characterized and a model has been developed, the accuracy of predictions made to evaluate remedy effectiveness, or contaminant fate-and-transport, depends upon the degree of successful calibration and verification of the model simulations. Errors in the model used for predictive simulations, even though small, can result in gross errors in solutions projected forward in time. Monitoring of hydraulic heads and groundwater chemistry provides the means to assess the accuracy of predictive simulations. The collection of these data during the remedial or corrective action is referred to as "performance monitoring." Performance monitoring verifies the predicted behavior of the hydrogeologic system through measurements of the actual behavior of the hydrogeologic system and establishes a way to understand exposure risks and to demonstrate compliance with environmental statutes. Field verification of the modeled simulations provides the evidence to support the conclusion of the model.

A model developer may want to compare the model predictions against the performance monitoring data and re-assess the conceptual model and model calibration. This process is referred to as a “post-audit.” Whether or not a post-audit is performed depends on whether the model has short- or long-term use. For long-term applications, a post-audit may be completed on a continuous basis as performance monitoring data are collected. Model conceptualization and calibration may be assessed and modified as needed to gain a better understanding of the physical and chemical processes within the aquifer system. In this application the revised model can be used in support of remedy optimization; however, even with post audits and continued improvement in the predictive capability of the model, appropriate field measurements and facility-specific information support the remedy effectiveness at the facility. Field verification of the model provides support in demonstrating remedy effectiveness.

[1]For the purpose of this technical resource document, the term “facility” is being used as a general reference to a property with environmental contamination and is not intended to be applied as it is statutorily defined in the Natural Resources and Environmental Protection Act (NREPA), PA 451 of 1994, as amended.

1.0 INTRODUCTION

The use of groundwater-flow models is prevalent in the field of environmental hydrogeology. Typically, models have been applied to predict the effectiveness of remedial or corrective actions or the fate-and-transport of contaminants for risk evaluation purposes. This document was developed by the Groundwater Modeling Program (GMP) in the MDEQ Remediation and Redevelopment Division (RRD), to assist in the application and development of groundwater-flow and solute-transport models, and the proper documentation and presentation of simulations for models that have been developed in support of remedial and corrective actions.

The scope of this document is to describe, in general terms:

- *Groundwater modeling concepts,*
- *Different types of models,*
- *Hydrogeological characterization needed to develop a model for a facility,*
- *Groundwater modeling procedures,*
- *Need for verification and performance-monitoring sampling,*
- *Appropriate level of model documentation, and*
- *Model review submittal procedures.*

It is not the intent of this document to provide a detailed discussion of all groundwater modeling concepts or procedures, or of particular groundwater model types. A list of selected references, which provide a more thorough discussion of the concepts presented in this document, is presented in Appendix A. Also, a number of technical terms are used throughout this document when describing various aspects of groundwater modeling. A glossary of these and other commonly used modeling terms and their definitions are contained in Appendix B. The reader is referred to both of these appendices, either to locate a source for more information concerning groundwater modeling or for definitions of groundwater modeling terms.

Finally, the discussion contained in this document reflects the types of models and scope of the model applications that are typically completed and submitted to MDEQ for department review. As an example, most submitted models are either one dimensional analytical fate-and-transport models or multi-dimensional finite-difference groundwater-flow or solute-transport models using automated trial-and-error calibration techniques. These models and their use are the primary focus of this document. There are other types of models (Analytic Element Method or Finite Element), automated calibration techniques (PEST or MODFLOWP), or post-audits whose application appears in the hydrogeological literature; however, these model or techniques have seldom been applied at facilities in Michigan. As a result, these models or techniques receive only brief mention in this document. The interested reader may refer to one or more of the selected references found in Appendix A.

2.0 GROUNDWATER MODELS

In general, models are conceptual descriptions or approximations that describe physical systems using mathematical equations – they are not exact descriptions of physical systems or processes. The applicability, or usefulness, of a model depends on how closely the mathematical equations approximate the physical system being modeled. In order to evaluate the applicability, or usefulness, of a model, a thorough understanding of the physical system and the assumptions embedded in the derivation of the mathematical equations will produce better predictions. A detailed discussion of the assumptions and derivations of the equations that are the basis of different groundwater models is beyond the scope of this document. The reader is referred to the references included in Appendix A for this information (see Konikow and Grove, 1977; Wang and Anderson, 1982; and Zheng and Bennett, 1995, among others).

Groundwater models describe groundwater-flow and fate-and-transport processes using mathematical equations that are based on certain simplifying assumptions. These assumptions typically involve the direction of flow, geometry of the aquifer, the heterogeneity or anisotropy of sediments or bedrock comprising the aquifer, the contaminant transport mechanisms, and chemical reactions. Because of the simplifying assumptions embedded in the mathematical equations and the many uncertainties in the values of data required by the model, a model provides predictions as an approximation and not an exact duplication of field conditions.

Groundwater models, however, even as approximations are a useful evaluation tool that groundwater hydrologists may use in support of a remedial or corrective action.

Typical model applications as evaluative tool:

- *Estimating and tracking the possible migration pathway of groundwater contamination,*
- *Design and evaluation of design of hydraulic containment and pump-and-treat systems,*
- *Design and evaluation of groundwater monitoring networks, or*
- *Estimation of the possible fate and migration of contaminants for risk evaluation.*

It is important to understand general aspects of both groundwater-flow and fate-and-transport models to ensure that the application, or evaluation, of these models may be performed correctly.

2.1 General Concepts

2.1.1 Groundwater-Flow Models

Groundwater-flow models are used to calculate the rate and direction of movement of groundwater through aquifers and confining units in the subsurface, and the exchange of groundwater between aquifers and sources and sinks, where groundwater is added or removed from the aquifer. These calculations are referred to as “simulations.” The simulation of groundwater-flow depends upon a thorough understanding of the hydrogeologic characteristics of the facility and the surrounding area.

A groundwater-flow model simulates the following processes:

- *Movement of groundwater through aquifers and confining layers,*
- *Addition of groundwater by sources such as precipitation, leakage from surface water bodies, injection wells, infiltration galleries, etc.,*
- *Removal of groundwater by sinks such as pumping wells, drains, surface water bodies, interceptor trenches, etc., or*
- *The change in hydraulic-head and hydraulic gradients as a result of the addition or removal of groundwater by sources and sinks.*

The outputs from groundwater-flow model simulations are the hydraulic-heads and groundwater-flow rates that are in equilibrium with the hydrogeologic conditions (hydrogeologic framework, hydrologic boundaries, initial and transient conditions, hydraulic properties, and sources or sinks) defined for the modeled area.

Through the process of model calibration and verification, discussed in later sections of this document, the values of the different hydrogeologic conditions are varied to reduce the disparity between the model simulations and field data, and to improve the accuracy of the model. The model can also be used to simulate possible future changes to hydraulic-head or groundwater-flow rates as a result of future changes in stresses on the aquifer system. These are referred to as "predictive simulations." These are discussed in later sections of this document. facility-specific information including the monitoring of hydraulic-heads, hydraulic gradients, and groundwater-flow rates (where appropriate) are useful to support predictive simulations using groundwater-flow models.

2.1.2 Fate-and-Transport Models

Fate-and-transport models simulate the migration and chemical alteration of contaminants as they move with groundwater through the subsurface. Fate-and-transport models rely on the development of a calibrated groundwater-flow model or, at a minimum, an accurate determination of the velocity and direction of groundwater-flow, which has been based on field data.

A fate-and-transport model may simulate the following processes:

- *Movement of contaminants by advection and diffusion,*
- *Spread and dilution of contaminants by dispersion,*
- *Removal, or release, of contaminants by sorption, or desorption, of contaminants onto, or from, subsurface sediment or rock,*
- *Addition or removal of contaminants by contaminant sources or sinks, and*
- *Chemical alteration of the contaminant by chemical reactions which may be controlled by biological processes or physical-chemical reactions.*

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

As with groundwater-flow models, fate-and-transport models should be calibrated and verified by adjusting values of the different hydrogeologic or geochemical conditions to reduce the disparity between the model simulations and field data. This process may result in a re-evaluation of the model used for simulating groundwater-flow if the adjustment of values of geochemical data does not result in an acceptable comparison with contaminant migration direction or rate. Predictive simulations may be made with a fate-and-transport model to predict the expected concentrations of contaminants in groundwater as a result of implementation of a remedial or corrective action. Monitoring of the groundwater chemistry supports predictive simulations using fate-and-transport models.

2.2 Types of Models

The equations that describe the groundwater-flow and fate-and-transport processes may be solved using different types of models. Some models may be exact solutions to equations that describe very simple flow or transport conditions (analytical model), some models may use exact solutions of equations that describe sources and sinks and other parameters that are solved together using the superposition principle (analytic element model), and others may be approximations of equations that describe very complex conditions (numerical models). Each model may also simulate one or more of the processes that govern groundwater-flow or contaminant migration, rather than all of the flow-and-transport processes. As an example, particle-tracking models such as MODPATH simulate the advective transport of contaminants but do not account for other fate-and-transport processes. In selecting a model for use at a facility, it is necessary to determine whether the model equations account for the key processes identified at the facility. Each model, whether it is a simple analytical model or a complex numerical model, may have applicability and usefulness in hydrogeological and facility evaluation. Appendix D lists the model software used by the GMP, the processes simulated by the model, and the appropriate use of that model.

2.2.1 Analytical Models

Analytical models are an exact solution of a specific, greatly simplified, groundwater-flow or transport equation. The equation is a simplification of more complex three-dimensional groundwater-flow or solute-transport equations. Prior to the development and widespread use of computers, there was a need to simplify the three-dimensional equations because it was not possible to easily solve these equations. Specifically, these simplifications resulted in reducing the groundwater-flow to one dimension and the solute-transport equation to one or two dimensions. This resulted in changes to the model equations that include one-dimensional uniform groundwater-flow, simple uniform aquifer geometry, homogeneous and isotropic aquifers, uniform hydraulic and chemical reaction properties, and simple flow or chemical reaction boundaries. Analytical flow models are typically steady-state and one-dimensional, although some groundwater-flow models are two dimensional and some contaminant transport models assume one-dimensional groundwater-flow conditions and simulate transient one-, two- or three-dimensional transport conditions.

Because of the simplifications inherent with analytical models, it is not possible to use them to account for field conditions that change with time or space. This includes variations in groundwater-flow rate or direction, variations in hydraulic or chemical reaction properties, changing hydraulic stresses, or complex hydrogeologic or chemical boundary conditions.

Analytical models may be best suited for the following applications:

- *Initial assessments where a high degree of accuracy is not needed,*
- *Designing data collection plans prior to beginning field activities,*
- *Assessment of well performance or impact of withdrawal from or injection to wells,*
- *Estimating fluxes at boundaries,*
- *An independent check of numerical model simulation results, or*
- *Facilities where field conditions support the simplifying assumptions embedded in the analytical models.*

Examples of common analytical model codes that might be used for groundwater-flow or fate-and-transport simulations are: any of the well-hydraulics models (e.g. Theis equation), the Domenico model, BIOSCREEN, or BIOCHLOR.

2.2.2 Analytic Element Method Models

Analytic Element Method (AEM) models are computer codes that do not require the model domain to be discretized into network of grid cells or elements. The only discretization involves representing surface-water features as arcs or polygons. The discharge potential for each of these arcs or polygons is represented by analytical solutions (elements) describing groundwater-flow or transport processes. AEM's superpose the exact solutions for each element resulting in a solution to a more complex groundwater-flow or solute-transport problem.

However, when compared to numerical models, there are limitations inherent with AEM models. These include developing models that are generally limited to steady-state, two-dimensional flow, and generally homogeneous aquifer properties. However, there have been modifications that allow for specific cases of transient flow (e.g. Theis solution for transient flow from wells), multi-aquifer flow (e.g. quasi-3D approach in which vertical flow between aquifers is simulated using a leakance factor), and discrete polygons having different aquifer properties.

AEM models have been used in a wide variety of applications, although the number of applications lags far behind the number of applications of analytical or numerical models.

Some of the applications where AEM models appear to be well suited include:

- *Capture zone or wellhead protection area delineation,*
- *Simulating regional steady-state groundwater flow in homogeneous single layer aquifers,*
- *Modeling local-scale flow or transport conditions, or*
- *Determining regional hydrogeologic boundary fluxes for numerical models,*

Examples of analytic element model codes that might be used for groundwater-flow or fate-and-transport simulations are SLAEM, MLAEM, GFLOW, WinFlow, WhAEM2000, MODAEM, and CZAEM. The reader is referred to Haitjema (1995), and Strack (1989, 1999, and 2003) (references are included in Appendix A under “Analytic Element Methods”) for a more thorough discussion of AEM models.

2.2.3 Numerical Models

Numerical models are capable of solving the more complex equations that describe groundwater flow and solute transport. These equations generally describe multi-dimensional groundwater flow, solute transport, and chemical reactions, although there are one-dimensional numerical models. Numerical models use approximations (e.g. finite differences, or finite elements) to solve the differential equations describing groundwater flow or solute transport. The approximations require that the model domain and time be discretized. In this discretization process, the model domain is represented by a network of grid cells or elements, and the duration of the simulation is represented by a series of time steps.

The accuracy of numerical models depends upon the accuracy of the model input data, the size of the space and time discretization (the greater the size of the discretization steps, the greater the possible error), and the numerical method used to solve the model equations.

Numerical models may be used to:

- *Simulate very simple one- or two-dimensional flow and transport conditions, which may just as easily be simulated using an analytical model,*
- *Model more complex two- or three-dimensional groundwater-flow and solute-transport problems,*
- *Simulate steady-state or transient groundwater flow or solute transport,*
- *Assess regional- or local-scale flow or transport,*
- *Estimate fluxes at simple or complex hydrogeologic boundaries, or*
- *Simulate problems which cannot be adequately described using analytical or AEM models.*

Examples of some of the more common numerical model codes are MODFLOW, BIOPLUME II, BIOPLUME III, MOC, SUTRA, and FEFLOW.

3.0 GROUNDWATER MODEL DEVELOPMENT PROCESS

The following figure (Figure 1) shows the recommended steps to follow in developing either a groundwater-flow or fate-and-transport model:

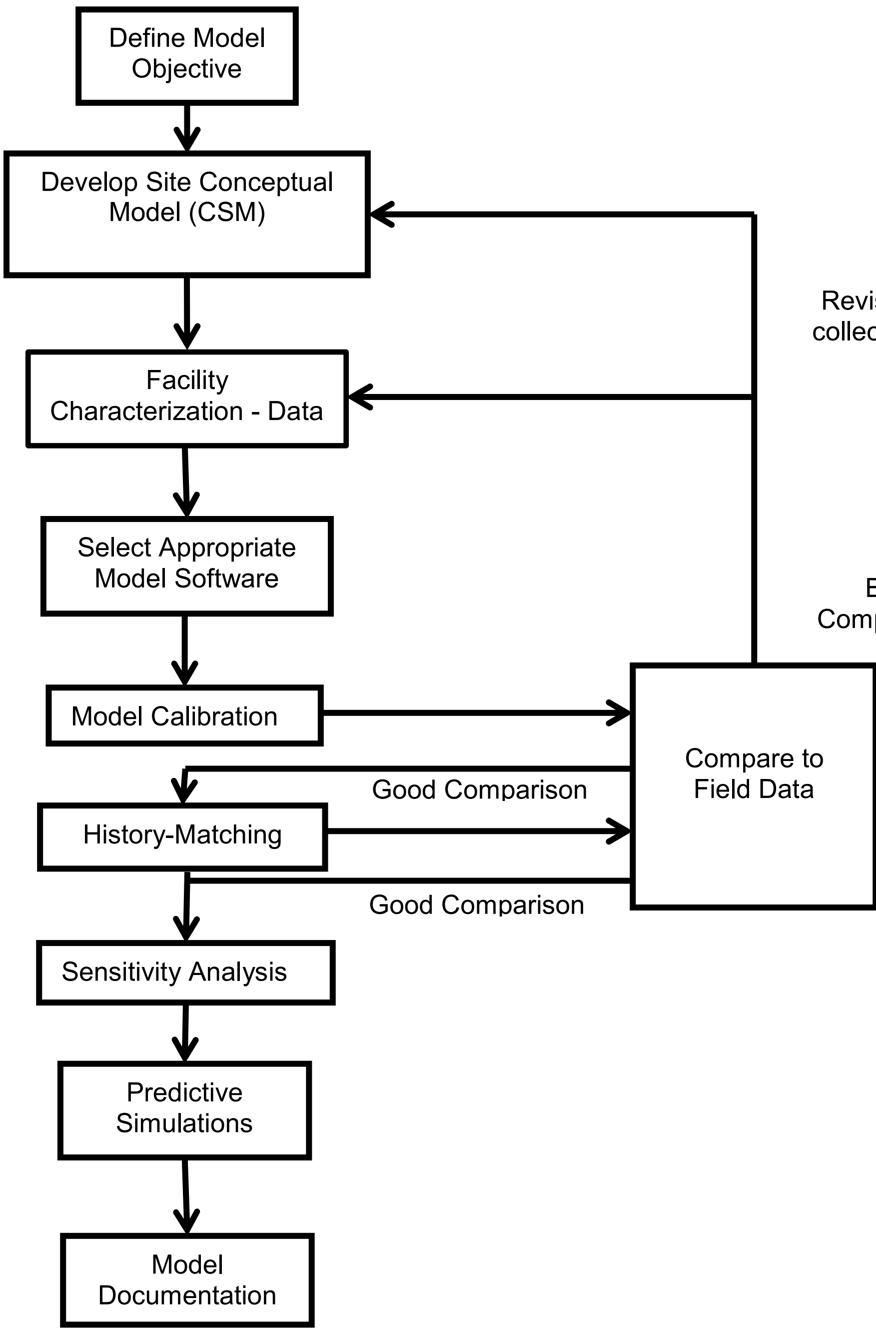

Figure 1 – Flow Chart Showing Model Development Process.

> **Note:** The Model Development Process should be followed whether developing a simple one-dimensional analytical model or a fairly complex multi-dimensional numerical model.

Each of the following sections describes, in more detail, the necessary elements of each of these steps in the model development process.

3.1 Purpose and Scope

The purpose and scope of the model application establishes the defined goals. That is, the model developer should identify the goals to be achieved by developing a model for the facility. They should also state the scope and limitations of the model.

3.2 Facility Characterization

Too often insufficient facility-specific data are collected prior to developing a model for a facility. The modeler often oversimplifies the conceptual model and relies on data derived from the literature or from other investigations without some demonstration that the data are even appropriate for conditions at the facility under investigation. Because of this, the conceptual model may not be representative of field conditions or fate-and-transport processes at the facility of interest, and the model developed for the facility may not accurately simulate groundwater-flow or contaminant fate-and-transport. Without proper facility characterization, it is not possible to select an appropriate model code or equation, or develop a model that can be used in the evaluation of remedial or corrective actions.

It is imperative that a thorough facility characterization be completed prior to developing a model. The modeler should base the model on as much facility-specific data as possible, rather than rely on literature-based values.

At a minimum, the facility characterization should provide the following hydrogeological information to be used in developing a groundwater-flow model:

- *Topographic data (including surface water elevations),*
- *Presence of surface water bodies and measured or estimated stream-discharge (base-flow) data,*
- *Other hydrologic boundaries (also referred to as boundary conditions), which control the rate and direction of groundwater movement,*
- *Regional geologic data, including well construction diagrams and soil boring logs depicting subsurface geology,*
- *Geologic cross sections and maps (if appropriate) drawn from soil borings and well logs, showing the subsurface extent and thickness of aquifers and confining units (hydrogeologic framework),*
- *Estimates of facility-specific hydraulic properties of the aquifers and confining units derived from aquifer tests, slug tests, or cores of aquifer and confining layer material,*
- *A description of the horizontal and vertical distribution of hydraulic head and hydraulic gradients throughout the modeled area, obtained from well measurements, for both beginning (initial conditions), equilibrium (steady-state conditions), and transitional conditions when hydraulic head may vary with time (transient conditions), if appropriate, and*

- *Distribution and magnitude of groundwater recharge, pumping or injection of groundwater, leakage to or from surface water bodies, etc. (sources or sinks, also referred to as "stresses"). These stresses may be constant (unvarying with time) or may change with time (transient).*

In addition to a thorough hydrogeological investigation, the simulation of fate-and-transport processes involves a complete characterization of the following:

- *Horizontal and vertical distribution of average linear groundwater velocity (direction and magnitude) determined by a calibrated groundwater-flow model or through accurate determination of direction and rate of groundwater-flow from field data,*
- *Identification of facility-specific contaminants (chemicals of concern),*
- *Horizontal and vertical distribution of contaminants,*
- *Direction and rate of contaminant migration,*
- *Identification of potential downgradient receptors,*
- *Location, history, dimensions, and mass loading or removal rate of chemicals by point sources or sinks,*
- *Boundary conditions for the solute (e.g. where groundwater and solutes enter or leave the model domain, other than point sources or sinks),*
- *Longitudinal, transverse, and vertical dispersivity (determined by calibrating fate-and-transport model to match the measured horizontal, transverse, and vertical spread of contaminants downgradient of source area),*
- *Distribution of electron acceptors, or transformation by-products,*
- *Equations describing facility-specific chemical transformation processes (determined by an examination of the distributions of chemicals of concern, electron acceptors, and transformation by-products),*
- *Facility-specific chemical decay rate or degradation constant (λ) (determined by an examination of the distribution and concentrations of the chemicals of concern and facility-specific recalcitrant chemicals),*
- *Effective porosity (η_e) or total porosity (η_T) of the aquifer(s) and confining layer(s), if applicable,*
- *Soil bulk density (ρ_b) of the aquifer(s) and confining layer(s) sediment, if applicable,*
- *Fraction of organic carbon (f_{oc}) of the aquifer(s) and confining layer(s) sediment, if applicable (determined through a sufficient number of analyses for total organic carbon to obtain a representative average), and*
- *Organic carbon/water partition coefficient (K_{oc}) for the chemical(s) of concern.*

These data should be collected at the facility between the source area and downgradient receptors. All information should be presented in map, table, and/or graph format in a report documenting model development.

It may not be possible to determine facility-specific values for all parameters used in fate-and-transport models (e.g. K_{oc}). When facility-specific values cannot be determined, it should be acceptable to use <u>conservative</u> values obtained from literature sources. However, it will be up to the investigator to provide:

- *The justification for using literature-derived values in place of facility-specific values,*
- *The literature citation from which the parameter value was derived, and*
- *A demonstration that the literature-derived value is appropriate for the facility.*

If literature-derived values are used, a sensitivity analysis provides the information that supports the applicability of all literature-derived values is essential. The use of a "bracket-analysis" using best and worst case values for these parameters should also be presented for all model predictive simulations to support applicability.

3.3 Model Conceptualization

Model conceptualization is the process by which data gathered during facility characterization are examined to determine relevant groundwater-flow and contaminant-transport processes at a facility. Completing the model conceptualization process is necessary prior to determining the modeling approach and which model software to use.

Questions to ask in developing a conceptual model include, but are not limited to:

- *Are there adequate data to describe the groundwater-flow directions at the facility?*
- *Are there adequate data to describe the distribution of the chemicals of concern at the facility?*
- *Can the groundwater-flow or contaminant transport be characterized as one-, two- or three-dimensional?*
- *Is the aquifer system composed of more than one aquifer, and is vertical flow between aquifers important?*
- *Is there recharge to the aquifer by precipitation or leakage from a river, drain, lake, or infiltration pond?*
- *Is groundwater leaving the aquifer by seepage to a river or lake, flow to a drain, or extraction by a well?*
- *Does it appear that the aquifer's hydrogeological characteristics remain relatively uniform, or do geologic data show considerable variation over the facility?*
- *Have the boundary conditions been defined around the perimeter of the model domain, and do they have a hydrogeological or geochemical basis?*
- *Do groundwater-flow or contaminant-source conditions remain constant, or do they change with time?*
- *Do chemical data show geochemical reactions taking place in groundwater, and are the processes understood?*
- *Are there receptors located downgradient of the known extent of the contaminant plume?*

Other questions related to facility-specific conditions may be asked in addition to those listed above. It is also necessary to assess the uncertainty in the answers to these questions. This conceptualization process and assessment of conceptualization uncertainties is necessary to decide on the modeling approach, and to determine which software to use in developing a model for the facility. The conceptualization process needs to be completed and described in the model documentation report.

3.4 Model Software Selection

After hydrogeological characterization of the facility has been completed, and the conceptual model developed, computer model software is selected. The selected model should be capable of simulating conditions encountered at the facility. The following general guidelines should be used in assessing the appropriateness of whether to use an analytical or numerical model, or whether the model should be capable of simulating one-, two-, or three-dimensional processes:

Analytical models should be used where:

- *Insufficient data are available to develop a more complex numerical model, and all that is necessary is an initial assessment of groundwater-flow or fate-and-transport processes,*
- *Field data show that groundwater-flow is primarily in one direction, or can be approximated as one-dimensional (e.g. along a streamline),*
- *Field data show that contaminant transport and geochemical processes are relatively simple and straightforward, and*
- *A screening of remedial alternatives for simple, idealized groundwater-flow and contaminant transport conditions is needed.*

Analytic Element Method models should be used where:

- *Field data show that groundwater-flow or transport processes can be represented by the superposition of analytical functions,*
- *Groundwater-flow and contaminant transport are generally horizontal within a single aquifer [although there are AEM models that can simulate multi-aquifer flow (e.g. MLAEM)],*
- *The aquifers are generally homogeneous (some AEMs may represent inhomogeneity using circular or elliptical zones of different hydraulic conductivity),*
- *Directions and rates of groundwater are generally in steady state and contaminant migration rates may change with time, and*
- *There may be multiple hydraulic or chemical sources and sinks.*

Numerical models should be used where:

- *Field data show that groundwater-flow or transport processes are relatively complex (although numerical models can be used very effectively to simulate relatively simple flow and transport conditions),*
- *Single or multiple aquifers are present,*
- *Horizontal and vertical movement of groundwater and contaminants is important,*
- *Directions and rates of groundwater and contaminant migration may change with time,*
- *There are multiple hydraulic or chemical sources and sinks, and*
- *Geochemical reactions may be relatively complex (e.g. electron-acceptor-limited reactions, multiple chemical species or electron acceptors).*

A one-dimensional groundwater-flow or transport model should be used primarily for:

- *Initial assessments where the complexity of groundwater-flow or solute transport processes is not known, or is assumed to be relatively simple,*
- *There is only one hydraulic or chemical source or sink located along the primary flow path from the source of contamination, and*
- *Facilities where a potential receptor is immediately downgradient of a contaminant source.*

Two-dimensional models should be used for:

- *Problems which include one or more groundwater sources/sinks (e.g. pumping or injection wells, drains, rivers, etc.),*

- *Facilities where the direction of groundwater-flow is obviously in two dimensions (e.g. radial flow to a well, or single aquifer with relatively small vertical hydraulic-head or contaminant concentration gradients),*
- *Facilities at which the aquifer has distinct variations in hydraulic properties,*
- *Contaminant migration problems where only the two-dimensional spread of the contaminant plume needs to be approximated (i.e., the thickness of the aquifer is small compared to the dimension of the area of interest and the vertical resolution of the contaminant plume is not important),*
- *There are hydraulic and chemical sources and sinks that are distributed laterally within the aquifer of interest, and*
- *Potential receptors are distributed laterally within the aquifer (i.e. not on a streamline passing through the source).*

Three-dimensional flow and transport models generally should be used where:

- *The horizontal and vertical movement of groundwater or contaminants is important,*
- *The hydrogeologic conditions are relatively well known,*
- *Multiple aquifers are present,*
- *There are hydraulic and chemical sources and sinks that are distributed laterally and vertically in one or more aquifers, and*
- *Potential receptors are distributed laterally and vertically in one or more aquifers.*

The rationale for selection of the appropriate model software should be discussed in the model documentation report. The choice of model software program for use at a facility is the responsibility of the modeler. Any appropriate groundwater-flow or fate-and-transport model software may be used provided that the model code has been tested, verified, and documented, and is accepted in the environmental-modeling community. However, if there are questions, it is recommended that the model developer contact the GMP at the beginning of the remedial investigation to discuss the selection of appropriate model software. A list of the model software currently used by the GMP is included in Appendix D. In the event that the software is not currently used by the GMP, and the software is not in the public domain, a copy of the software must be provided to the GMP, along with the program document and model documentation report, if review is required or requested. This includes analytical models that have been programmed in spreadsheets.

3.5 Model Calibration

Model calibration consists of changing the values of model input parameters, within a reasonable range, in an attempt to match a given aquifer hydraulic state or solute behavior within some acceptable criteria. This necessitates that field conditions at a facility be properly characterized. Lack of proper characterization may result in a model that is “calibrated” to a set of conditions which is not representative of actual field conditions. The calibration process typically involves calibrating to both steady-state and transient conditions. With steady-state simulations, there are no observed changes in hydraulic head or contaminant concentration with time for the field conditions being modeled. Transient simulations involve the change in hydraulic-head or contaminant concentration with time (e.g. aquifer test, an aquifer stressed by a well-field, or a migrating contaminant plume). These simulations are needed to narrow the range of variability in model input data, since there are numerous choices of model input data values which may result in similar steady-state simulations. Models may be calibrated without simulating steady-state flow conditions, but not without some difficulty.

At a minimum, model calibration should include comparisons between model-simulated conditions and field conditions for the following data:

- *Hydraulic head data,*
- *Hydraulic-head gradient (magnitude and direction),*
- *Water mass balance,*

And for fate-and-transport models:

- *Solute concentrations,*
- *Contaminant migration rates,*
- *Contaminant migration directions, and*
- *Degradation rates.*

These comparisons should be presented in maps, tables, and/or graphs. Each modeler and model reviewer will need to use their professional judgment in evaluating the calibration results. There are no universally accepted "goodness-of-fit" criteria that apply in all cases. However, it is important that the modeler make every attempt to minimize the difference between model simulations and measured field conditions. Typically, the difference between simulated and actual field conditions (residual) should be less than ten percent of the variability in the field data across the model domain. Errors should be randomly distributed, such that model results are not biased high or low within particular regions or over the entire model domain.

The modeler also should avoid the temptation of manually adjusting model input data on a scale that is smaller than the distribution of field data. This process results in a model that appears to be calibrated, but has been based on a set of model parameters that may not be supported by field data.

It also is very important that the modeler use all available information when calibrating a model. As an example, a model is not calibrated if the normalized head residuals are less than ten percent, but the model does not accurately simulate the magnitude and direction of hydraulic-head gradients, or contaminant migration directions.

Finally, a "calibrated" model having a residual error less than ten percent should not be considered accurate and without error.

3.6 History-Matching

A second step in the calibration process is the "history-matching" process. This process has been referred to by others as "model verification." A calibrated model uses selected values of hydrogeologic parameters, sources and sinks, and boundary conditions to match field conditions for selected calibration time periods (either steady-state or transient). This choice of "calibrated" model parameters is referred to as a "realization." However, the choice of the parameter values and boundary conditions used in the calibrated model is not unique. There may be an infinite number of statistically-similar realizations that give very different predictive model results. History-matching uses the calibrated model to reproduce a set of historic field conditions, other than those used in the initial model-calibration process, in an attempt to reduce the number of realizations and variability in simulation results.

The most common history-matching scenario consists of reproducing an observed change in the hydraulic head or solute concentrations over a different time period, typically one that follows the calibration time period. The best scenarios for model verification are ones that use the calibrated model to simulate the aquifer under stressed conditions. The process of model verification may result in the need for further refinement of the model. After the model has successfully reproduced measured changes in field conditions for both the calibration and history-matching time periods, it is ready for predictive simulations.

3.7 <u>Sensitivity Analysis</u>

A sensitivity analysis is the process of varying model input parameters over a reasonable range (range of uncertainty in values of model parameters) and observing the relative change in model response. Typically, the observed changes in hydraulic head, groundwater-flow rate, or contaminant transport (migration rate and concentrations) are noted. The purpose of the sensitivity analysis is to demonstrate the sensitivity of the model simulations to uncertainty in values of model input data. The sensitivity of one model parameter relative to other parameters is also demonstrated. Some common parameter estimation programs (e.g. PEST, MODFLOWP) incorporate a quantitative analysis of parameter sensitivity as part of the parameter estimation output.

A sensitivity analysis may be performed at any point in the model development process. Perhaps the greatest utility of a sensitivity analysis is in determining the direction of future data-collection activities. Parameters for which the model is relatively sensitive could necessitate additional characterization; model-insensitive parameters would not necessitate further field characterization. It is also useful to conduct a sensitivity analysis during predictive simulations to demonstrate the impact of varying pertinent model parameters on the simulation outcome.

3.8 <u>Parameter Estimation</u>

The previous three sections (**<u>Model Calibration</u>**, **<u>History-Matching</u>**, and **<u>Sensitivity Analysis</u>**) describe general concepts that apply whether using a non-automated or automated method of estimating parameter values for calibrating a model. Automated methods (referred to as “Parameter Estimation” or “Inverse Modeling”) make use of techniques such as nonlinear least-squares regression, as an example, to calibrate a model by adjusting model parameters to minimize the difference between measured and simulated hydraulic-heads and groundwater-flow rates. This is the same objective as the non-automated trial-and-error approach.

The advantages of using automated methods are that:

- *The method quickly determines a best fit of model parameters that meet the modelers calibration criteria,*
- *The quality of the calibration may be quantified,*
- *Data deficiencies are identified, and the need to collect or the worth of additional data may be quantitatively assessed,*
- *Confidence limits may be placed on parameter values or model predictions,*
- *Parameter sensitivities are determined,*
- *Extreme model parameter correlation may be identified, and*
- *Provide a means of quantitatively comparing alternate conceptual models.*

Some of the more common parameter estimated computer programs used are PEST, MODFLOWP, and UCODE. The reader is referred to Doherty (2002), Hill (1992), or Poeter and Hill (1998) (references listed under "Parameter Estimation" in Appendix A) for a more thorough description of these computer codes and the methods used for parameter estimation.

4.0 PREDICTIVE SIMULATIONS

Predictive simulations may be used to estimate the hydraulic response of an aquifer, the possible migration pathway of a contaminant, the contaminant mass removal rate from an aquifer, or the concentration of a contaminant at a point of compliance at some future point in time. The predictive simulations are estimates, not certainties, to aid the decision-making process. As an example, the design of a groundwater remediation system may be based on predictive model simulations. A model may be used to predict the number of extraction wells and pumping rates needed to capture a contaminant plume and to estimate the contaminant concentration of the extracted groundwater. Monitoring of hydraulic heads and contaminant concentrations are then used to verify hydraulic containment and remediation of the contaminant plume.

Predictive simulations are based on the conceptual model developed for the facility, the values of hydrogeological or geochemical parameters used in the model, and on the equations solved by the model software. Errors in values of model parameters, or differences between field conditions and the conceptual model or model equations will result in errors in predictive simulations. Models are calibrated by adjusting values of model parameters until the model response closely reproduces field conditions within some acceptable criteria, in an attempt to minimize model error. However, the time period over which a model is calibrated is typically very small, especially when compared to the length of time used for predictive simulations. Relatively small errors observed during the time period over which the model calibration or history-matching was performed may be greatly magnified during predictive simulations because of the greater time period length typically used in predictive simulations. The growth in errors resulting from projecting model stimulations into the future need to be evaluated by monitoring field conditions over the time period of the predictive simulation, or until appropriate cleanup criteria have been achieved.

Because even a well-calibrated model is often based on insufficient data or oversimplifications, there will be errors and some degree of uncertainty in predictive models. For this reason, all model predictions should be expressed as a range of possible outcomes that reflect the uncertainty in the most sensitive model parameter values. As an example, model predictions should be presented using a "bracketing-type" analysis in which the range of model input parameters are varied from least conservative to most conservative, rather than presenting a single model prediction. In addition, the final predictive simulations on which remedial decisions are based should be conservative. That is, given the uncertainty in model input parameters and the corresponding uncertainty in predictive model simulations, model simulations which result in a reasonable "worst-case" simulation should form the basis of design. Facility-specific data should be used to support a more reasonable worst-case scenario. Or stated another way, facility-specific data should be collected to limit the range of uncertainty in predictive models so that "worst-case" simulations are not unreasonable.

5.0 MODEL PREDICTIONS AND PERFORMANCE MONITORING

Once calibrated, a groundwater-flow or fate-and-transport model may be applied to evaluate changes in a number of different hydrogeologic or chemical conditions at environmental contamination facilities. Some of the typical model applications are to predict the change in hydraulic-heads or groundwater-flow directions as a result of changes in hydraulic stresses (e.g. increases in pumping rates, etc), evaluate the effectiveness of a remedial or corrective action, or estimate the migration pathway and concentrations of contaminants in groundwater. However, errors in the model, even though small, can result in gross errors in solutions projected forward in time. It is for this reason that, in addition to remedy assessment, performance monitoring is useful to compare future field conditions with model predictions to assess model error.

A model may be considered part of the facility compliance requirements if specified as part of a response activity plan, corrective action plan (CAP), or negotiated settlement. However, a model cannot provide verification of remedy effectiveness (e.g., hydraulic containment of a contaminant plume or estimation of the chemical concentration at the point of human or environmental exposure). At best, a model can only provide an estimate of the relative effectiveness of a remedial or corrective action. Verification of actual performance can only be demonstrated by the measurement of appropriate field data. Performance monitoring provides the means of physically measuring the actual behavior of the hydrogeologic system and demonstrating compliance with environmental statutes. This is consistent with the Risk Based Corrective Action (RBCA) process. ASTM guidelines state that "Predictive modeling is not used in the RBCA process as a substitute for site-specific verification data" (ASTM Standard E 1739-95 (2002), Appendix X3.4.3).

The degree of performance monitoring at a facility depends on the conditions or actions that have been simulated and the associated level of risk to the downgradient receptors. With any performance monitoring plan and network, there should be a sufficient number of sampling locations that are properly distributed to verify model simulation results. Monitoring wells that are installed to investigate the possible extent of a contaminant plume often are not appropriately located to monitor the performance of a remedy. For this reason, it is very likely that additional nested monitoring wells (individual wells screened at different vertical depths) may be needed to support remedy performance effectiveness and model simulation results.

Examples of model simulation outcomes and the important elements of an effective performance monitoring plan are contained in the following sections.

5.1 Hydraulic Containment

A model simulating effective hydraulic containment of a contaminant plume by a pump-and-treat system, for a given constant pumping rate, should show the following:

- *Simulated hydraulic gradients toward the extraction wells over an area greater than the delineated extent of contamination, and*
- *Simulated declining chemical concentrations in monitoring wells located downgradient of the simulated extent of capture shortly after the establishment of the capture zone.*

A performance monitoring plan to verify model predictions and remedy effectiveness includes the following:

- *Monitoring of pumping rates to make sure that actual pumping rates are equal to, or exceed, those used in the model.*
- *Measurement of hydraulic-head in all monitoring wells to show hydraulic gradients toward the extraction wells over an area larger than the delineated extent of contamination. Additional piezometers or monitoring wells should be installed if a sufficient number of wells are not available to measure heads, especially between the extraction wells and the downgradient*

extent of capture. Pumping wells do not provide appropriate water level measurements in this case.

- *Collection of groundwater samples in monitoring wells located beyond the simulated extent of capture. Chemical concentrations in groundwater at these points should show a declining trend with time. Additional monitoring wells may need to be installed if there is not a sufficient number of monitoring wells properly located immediately beyond the downgradient extent of capture.*

5.2 Contaminant Removal

Some remedial or corrective actions may include removal of contaminated groundwater to reduce the overall chemical concentrations within the plume. Model simulations of an effective contaminant removal remedy should show the following:

- *An overall declining trend in chemical concentrations within the delineated extent of groundwater contamination, and*
- *Declining chemical concentrations at locations beyond the downgradient extent of the zone of contaminant removal, and*
- *No increase in chemical concentrations at locations where previous sampling had indicated no detectable or very low detectable concentrations of facility-specific chemicals.*

A proper performance monitoring plan to verify model predictions and remedy effectiveness consist of the following:

- *Monitoring of pumping rates to make sure that actual pumping rates are equal to, or exceed, those used in the model.*
- *Collection of groundwater samples from the extraction system. Chemical concentrations in extracted groundwater and the mass of chemicals removed by the extraction system should show a declining trend with time.*
- *Collection of groundwater samples in monitoring wells located within the delineated extent of the contaminant plume. Overall, the concentrations of chemicals in groundwater should show a declining trend with time.*
- *Collection of groundwater samples in monitoring wells located beyond the simulated extent of capture or at a compliance boundary. In locations where groundwater contamination exists, chemical concentrations in groundwater at these points should show a declining trend with time. At the compliance boundary, chemical concentrations in groundwater should not show concentrations that exceed applicable compliance criteria. Additional monitoring wells need to be installed if an insufficient number of monitoring wells are located, and evenly distributed, immediately beyond the downgradient extent of contaminant removal.*

5.3 Natural Attenuation

Model simulations of an effective natural attenuation remedy should show that the contaminant plume is stable or shrinking through the following:

- *Declining concentrations of the chemicals of concern in all monitoring wells located within the delineated extent of groundwater contamination,*
- *Declining concentrations in appropriate electron acceptors where degradation is the primary attenuation mechanism,*

- *Increasing concentrations of degradation by-products where degradation is the primary attenuation mechanism, and*
- *No increase in chemical concentrations in monitoring wells located beyond the delineated extent of the stabilized contaminant.*

Facilities at which natural attenuation has been simulated warrant extensive monitoring of appropriate chemical parameters and hydraulic-heads. A proper performance monitoring plan to verify model predictions and remedy effectiveness consists of the following:

- *Collection of groundwater samples from all performance monitoring wells located within the contaminant plume and screened at appropriate intervals within the aquifer. Samples should be analyzed for all appropriate chemicals of concern, degradation by-products, and appropriate field parameters. Chemical monitoring should be necessary at a sufficient number of locations to evaluate the migration or mass removal of contaminants. Sample results should compare well with simulation results.*
- *Collection of groundwater samples from all performance monitoring wells screened at appropriate depths located beyond the downgradient extent of the contaminant plume. Samples should be analyzed for all appropriate chemicals of concern, degradation by-products, and appropriate field parameters. Chemical monitoring should be at a sufficient number of locations to evaluate the potential for downgradient migration of contaminants. Sample results should compare well with simulations results and show no downgradient migration of chemicals of concern above appropriate compliance criteria.*
- *Hydraulic-head measurement horizontally and vertically is necessary to verify groundwater and contaminant migration directions.*
- *Additional monitoring wells need to be installed if an insufficient number of monitoring wells are located, and evenly distributed, within, and along the horizontal and vertical migration path of the contaminant plume, and immediately beyond the downgradient extent of the stabilized contaminant plume at appropriate depths within the aquifer.*

Further details on monitoring natural attenuation are contained in RRD Operational Memorandum No 4, Attachment 8, Monitored Natural Attenuation.

5.4 Potential Impact to Downgradient Receptors

Models may be used to show the potential for impact to downgradient receptors such as potable water supply wells or surface water bodies (e.g. lakes and streams). The simulation results should show the following:

- *Concentration distribution between the contaminant source area and the downgradient receptor.*
- *The expected concentration at the downgradient receptor.*

A properly-designed performance monitoring plan to verify the model consists of the following:

- *Collection of groundwater samples from all wells located between the contaminant source area and the downgradient receptor. These wells should be located along and perpendicular to the primary migration path of the contaminant plume. Samples should be analyzed for all appropriate chemicals of concerns, pertinent degradation by-products, and appropriate field parameters. Chemical monitoring should be at a sufficient number of horizontal and vertical*

locations to evaluate the migration rate, dispersion, or mass removal rate of contaminants. Sample results should compare well with simulation results.
- *Collection of groundwater samples along a compliance boundary upgradient of the receptor. Samples should be analyzed for all appropriate chemicals of concern, pertinent degradation by-products, and appropriate field parameters. Chemical monitoring should be at a sufficient number of horizontal and vertical locations to evaluate the potential impact to the receptor. Sample results should compare well with simulation results.*
- *Hydraulic-head measurements are necessary to verify groundwater and contaminant migration direction.*
- *Additional monitoring wells need to be installed if an insufficient number of monitoring wells are located, and evenly distributed within, and along the migration path of the contaminant plume, and along a compliance boundary upgradient of the receptor.*

5.5 Impact on Surrounding Hydrology

A model may also be used to simulate the impact of pumping from a groundwater-extraction well on the hydrology of nearby surface water bodies, wetlands, or groundwater levels within the same or adjacent aquifers. Model simulations might show the following:

- *Simulated declines in groundwater levels in the region surrounding the extraction well, and*
- *Simulated decrease in groundwater discharge rates to surface-water bodies or wetlands, or an increase in groundwater recharge rates from surface-water bodies or wetlands.*

A proper performance monitoring plan to verify model predictions for assessing the impact of a groundwater extraction well consists of the following:

- *Monitoring of pumping rates to make sure that actual pumping rates are equal to those used in the model.*
- *Measurement of hydraulic-head(s) in all monitoring wells and stage elevations in surface-water bodies or wetlands, if applicable, prior to the beginning of groundwater extraction to show "base-line" water level conditions. Additional piezometers, monitoring wells or staff gages may be needed if there are not a sufficient number of wells or staff gages available to measure water levels on a regional basis, especially between the extraction well(s) and the nearest areas of potential conflict. The areas of potential conflict might be existing groundwater-supply wells, surface-water bodies, or wetlands.*
- *Measurement of hydraulic-heads in all monitoring wells and stage elevations in surface-water bodies or wetlands, if applicable, after the beginning of groundwater extraction to show the impact of groundwater pumping on regional water levels. These data should be collected on a regular basis, for a sufficiently long time period, to show the long-term impact of development on water levels.*
- *It is also beneficial to locate monitoring points in areas beyond the expected zone of influence (ZOI) of the extraction well. Water levels should be measured at these points before and after groundwater pumping has begun. The purpose of these monitoring points is to determine background fluctuations in water levels so that such fluctuations might be "removed" from the performance monitoring data.*

6.0 MODEL POST AUDITS

Following model calibration, predictions are made with the model assuming that the cause-and-effect relationship between stresses and aquifer response are accurately characterized in the model. However, this assumption is seldom correct since there are typically too few data representing a relatively-short time interval with which to characterize the hydrogeology or to calibrate the model. Also, the physical or chemical processes taking place in the aquifer system have been overly simplified in the model; and, predicted stresses on the aquifer system and the impact of boundary conditions may differ significantly from past or present conditions. Results reported in the literature show that these model "shortcomings" often result in predictive simulations that do not compare well with field data collected at the facility. At this point in the project, a modeler may want to compare the model predictions against the performance monitoring data and re-assess the conceptual model and model calibration. This process is referred to as a "Post-Audit."

Whether or not a post audit is performed depends on the intended short- and long-term use of the model. For many facilities a model is used either for remedy-screening or design purposes. In these cases, it may not be necessary to perform a post audit since remedy effectiveness will be assessed and remedy modifications will be made on the basis of performance monitoring data and not model simulations. There are a relatively few, larger-scale facilities for which a model may be developed for long-term use. In these applications, a post-audit may be completed on a continuous basis as performance monitoring data are collected. Model conceptualization and calibration may be assessed and modified as needed to gain a better understanding of the physical and chemical processes within the aquifer system. If, after several post-audits, it can be demonstrated that the model is capable of accurately simulating flow and transport conditions within the aquifer system of interest, the model, along with the field data, may be used to optimize the performance monitoring network. However, even with post-audits and continued improvement in the predictive capability of the model, remedy effectiveness will be based on the monitoring data collected at the facility. The model, no matter how much it has been improved, cannot be used to demonstrate remedy effectiveness.

7.0 DOCUMENTATION OF GROUNDWATER-FLOW AND FATE-AND-TRANSPORT MODELS

A groundwater model developed for a facility, whether an analytical or numerical model, should be described in sufficient detail so that the model reviewer may determine the appropriateness of the model for the situation that is simulated. Submittals that require or request MDEQ approval need to include a model documentation report and model datasets (in digital format).

7.1 Report

Groundwater modeling documentation needs to provide a problem definition, present conceptualization of the facility hydrogeology, and the data or information used to develop this conceptualization, and detail the process by which the model was selected, developed, calibrated, verified and utilized. A report documenting the development and application of the model should be presented to the MDEQ for review. The report should include all data used in developing and calibrating the model, and the results of all pertinent model simulations. This information should be included in text, table, and figure format. A suggested report format is described in Appendix C.

Additional information may be necessary in the model documentation report. Examples are work plans for additional facility characterization where model simulations show data deficiencies, or groundwater monitoring plans, proposals, or recommendations to collect data needed to verify model predictions. Other data may be required, depending on the conditions at the facility. These additional subjects should be addressed within the body of the report. This may require additional figures and tables, or report sections.

7.2 Model Review Submittal Procedures

Any model simulations upon which remedial decisions are made, need to be verified, rather than simply accepted. This process of verification and review of groundwater-flow and solute-transport models is performed by the GMP, along with district staff in the MDEQ, RRD. A copy of the model dataset in digital format should be provided as part of model documentation by the party responsible for developing the model. The datasets for the different simulations (model calibration, history-matching and predictive simulations) should be provided and clearly labeled. If a model is used that is proprietary and not currently supported by the GMP, it may be necessary for the modeler to provide a copy of the model software for model review purposes only. The copy of this model software will be returned after model review has been completed.

Appendix A.

Frequently Asked Questions Regarding the Application of Analytical Fate and Transport Models for Natural Attenuation

This document is provided as an addendum to the Groundwater Modeling Resource(GMR). That guidance describes the appropriate use of models that are developed in support of remedial decisions at facilities with groundwater contamination. It is intended that the concepts and guidelines described in the GMR be used whether the model is a complicated three-dimensional groundwater-flow and solute-transport model or a simple analytical model. At such facilities, very simple fate-and-transport models have commonly been applied to predict contaminant concentrations downgradient of the contaminant-release area for natural attenuation remedies or to evaluate the potential impact to downgradient receptors such as surface-water bodies or potable water supply wells.

In order to effectively apply these simple analytical models it is important that: the facility be properly characterized so that the proper analytical model equation may be selected and model parameter values be estimated from facility-specific data; the model developer understand the assumptions and limitations of the particular equation that is being solved; an attempt is made to demonstrate model calibration and accuracy; and to present model predictions as a range of possible outcomes. These concepts are all discussed in the GMR.

The following series of questions and answers should provide the necessary clarification to properly use simple fate and transport models in support of natural attenuation remedies.

What is fate-and-transport modeling?

Fate and transport modeling is the estimation of chemical concentrations dissolved in groundwater down gradient of a contaminant source.

What are the most commonly used fate-and-transport models?

By far, the majority of fate-and-transport models that are used to support natural attenuation remedies are simple analytical equations that have been programmed in a spreadsheet. Some of the most commonly used public domain spreadsheet programs are BIOSCREEN (Newell and others, 1997), BIOSCREEN-AT (Karanovic and other, 2007), and BIOCHLOR (Aziz and others, 2000). Many model developers program the steady-state attenuation equation found in Table X3.1 in the Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites (ASTM, 1996). These equations are generally based on the analytical flow and transport model developed by Dr. P. A. Domenico (Domenico and Robbins, 1985).

What natural attenuation processes can be simulated with a fate-and-transport model?

That depends on the equation that is solved by the model. All models simulate the movement of contaminant with the groundwater (advection), the spreading of contaminants as they move with the groundwater (dispersion), simple sorption or desorption of the contaminants to or from sediments (retardation), and simple exponential removal of contaminant by chemical or biological means (decay or degradation). All models simulate the fate-and-transport of a single chemical. Complex numerical models can simulate the transport and chemical interaction of multiple chemicals.

When should fate-and-transport modeling be conducted at a facility?

Fate-and-transport modeling can be applied at any time during an investigation at a facility. Using a model during the facility investigation can be very useful in guiding further data collection activities or in the design of monitoring well networks. In this example, facility characterization is not complete, and model predictions should be viewed as gross approximations. In contrast, the application of fate-and-transport models to assess the effectiveness of a proposed remedial or corrective action necessitates that proper facility characterization be completed beforehand.

What are the most common errors or shortcomings observed in fate-and-transport model applications submitted to MDEQ?

The following is a list of the most typical shortcomings or errors that are observed the analytical fate and transport model that are submitted to MDEQ. These are grouped into three general categories: 1) Facility Characterization, 2) Model Selection and Application, and 3) Remedy Performance Monitoring.

Facility Characterization:

- *Contaminant source dimensions and concentrations not properly characterized potentially resulting in an underestimation of the contaminant mass being released to the groundwater.*
- *Horizontal and vertical extent of contaminant plume not properly determined (e.g. too few or widely-spaced wells, or inadequate vertical profiling of the contaminant plume).*
- *Groundwate-flow direction not adequately defined (e.g. too few or widely-spaced wells, especially near compliance boundaries).*
- *As a result, the migration direction of the plume center of mass is not correctly delineated and monitoring wells are not placed along the plume centerline to aid in model calibration or to monitor natural attenuation.*

Model Selection and Application:

- *Models are not developed following standard modeling guidelines whether using an analytical or numerical model. For specific guidelines related to the use of an analytical fate-and-transport equation for Risk-Based Corrective Actions, the model developer is referred to section X3.7, Procedures for Predictive Migration Models, in ASTM (1996).*
- *Models do not show through the presentation of facility data and development of a conceptual facility model that the analytical model or equation solved by the analytical model is applicable to the facility being investigated.*
- *The "Domenico" model equation is the most commonly used analytical fate-and-transport model equation; however, there is a lack of understanding that there are different versions of the "Domenico" model equation. The differences are based on the location of the contaminant source within the aquifer and the directions of vertical dispersion that are simulated. That is, there is a version of the "Domenico" equation for: 1) a source at the*

water table in which only downward vertical dispersion is allowed, 2) a source that is located at the midpoint of the aquifer and vertical dispersion in the upward and downward direction is allowed, and 3) there is no vertical dispersion, either because contaminant is spread vertically over the entire aquifer thickness, or there are hydrogeological constraints on vertical dispersion. The different forms of the "Domenico" model equation are described in detail in Domenico and Robbins (1985) and Domenico (1987). The steady-state attenuation equation shown in Table X3.1 of the Standard Guide for Risk-Based Corrective Action (RBCA) Applied at Petroleum Release Sites (ASTM, 1996) assumes that the center of the contaminant source is located at the mid-point of the aquifer allowing both upward and downward vertical dispersion of the plume. This is the equation used by many consultants and may not be applicable for many of the Part 213 LUST sites where the contaminant source is located at the water table. The associated text in this document does not discuss the limitations, or appropriate use, of the equation shown in Table X3.1. It is the responsibility of the model developer to demonstrate, through proper contaminant plume delineation, which equation to use. The selection of the appropriate model equation or value for vertical dispersivity is often not aligned with the vertical spread of the contaminant plume observed in the field

- *The model seldom compares the simulated plume width to the plume width delineated in the field.*

- *There is seldom an attempt to calibrate the model, regardless of the model or equation that has been selected. During model calibration, the model developer demonstrates through a comparison between model-simulated concentrations and contaminant plume width to those measured in the field that the model can reasonably reproduce field conditions. This is a necessary step in which the model developer demonstrates that the model may be a reasonable predictor of contaminant fate-and-transport.*

- *When there is an attempt to calibrate a model (e.g. to estimate degradation rates), problems arise from not using data from monitoring wells located along the plume migration centerline. The result is usually an overestimation of the rate of attenuation and an underestimation of contaminant concentrations downgradient of the source area.*

- *Predictions made with fate-and-transport models rarely attempt to show the impact of parameter uncertainty on predicted contaminant concentrations downgradient of the source area or at the compliance boundary. <u>The predicted contaminant concentrations should be presented as a range of possible concentrations</u>.*

<u>Performance Monitoring:</u>

- *Because of inadequate facility characterization and downgradient determination of groundwater flow directions and contaminant extent, monitoring wells and screens are not properly located along the plume migration pathway or at compliance boundaries.*

When should fate-and-transport models be included in a Part 213 FAR or Part 201 RAP?

Consultants should not submit a Part 213 Final Assessment Report (FAR) or Part 201 Response Activity Plan (RAP) that contains a fate and transport model, unless the site characterization [Section 21311a(1)a and Section 20114(1)a], and a monitoring plan [Section 21309a(2)c and Section 20118(10)a-c] are acceptable to the MDEQ, and the necessary steps for completing a reliable fate-and-transport model have been followed.

What is acceptable, or proper, facility characterization for fate-and-transport model application?

Acceptable, or proper, facility characterization for appropriate fate-and-transport model application consists of complete determination of the following elements:

- *Source dimensions (area and thickness), chemicals comprising the source of contamination (chemicals of concern), and concentrations of the chemicals within the source area remaining on the facility. This includes soil returned to tank cavities with or without characterization.*

- *Horizontal and vertical direction of groundwater migration and an analysis of the possible variation with each measured over time.*

- *Rate of groundwater migration through the measurement of hydraulic conductivity and hydraulic-head gradient.*

- *Nature and extent of groundwater contamination, both horizontally and vertically, at the source area and downgradient of the source area as determined by vertical aquifer sampling. Placement of permanent two-inch-diameter nested monitoring wells should occur where appropriate.*

- *Specific attention should be given to the vertical delineation of MTBE, especially downgradient of any places where the uppermost aquifer may receive significant recharge over a relatively-small area (e.g., stormwater-retention basins, septic fields, dry wells, or natural features).*

- *Identification of all potential receptors downgradient from the source area (e.g. public or private water-supply wells, residences with basements, surface-water bodies, etc.) needs to be completed.*

Without proper facility characterization it is not possible to calibrate the fate-and-transport model, or assess whether the model predictions are reasonable, acceptable, or useful for evaluating risk-based closure options.

What are the necessary steps to developing a reliable fate and transport model?

A model developer should use the information provided in this document whether using an analytical or numerical model. For specific information related to the use of the “Domenico” equation for Risk-Based Corrective Actions, the model developer is referred to section X3.7, Procedures for Predictive Migration

Models, in ASTM (1996). General steps for developing and documenting a fate and transport model are as follows:

- *Present in map view, the horizontal extent of the contaminant plume. In more than one cross-section view, present the vertical extent of the plume, along and perpendicular to the plume migration pathway/centerline. On the map, define the plume centerline and cross-section lines.*

- *Determine that the model used to analyze natural attenuation is appropriate for the facility. That is, evaluate whether model assumptions are consistent with field conditions. For example:*

    - *Can groundwater-flow be characterized as a uniform, one-dimensional flow in a single aquifer with isotropic, homogeneous hydraulic and geochemical properties? Since this is seldom the case, model predictions should always be presented as a range of possible outcomes that reflect the difference between the assumed ideal conditions and field conditions.*
    - *Can the source be represented as a continuous infinite or decaying source of contaminants?*
    - *Can the geochemical reactions be approximated by a simple decay equation?*

- *Where possible, determine the values of model input parameters through facility investigations. All data collected during facility investigations should be placed on maps or cross sections. For parameters that are not easily measured in the field, (e.g., soil bulk density) <u>conservative</u> values from the literature may be used. <u>The model developer should provide documentation for all values derived from the literature</u>. The following is a list of typical parameters used in simple fate-and-transport model and the MDEQ-recommended means of obtaining parameter values.*

    - *The volume of contaminated soils remaining in the source area – Determined through soil borings and chemical analysis of the soils.*
    - *Hydraulic gradient – Determined from static-water-level measurements in monitoring wells.*
    - *Hydraulic conductivity – Derived from slug tests or aquifer tests conducted in facility monitoring wells.* ***Slug tests results need to be evaluated to determine if they are consistent with aquifer materials known to exist at the facility. Documentation of the evaluation should be provided.***
    - *Effective porosity – May be estimated from drainable porosity measurements of soil or sediment core sample, or use a range of values derived from the literature.*
    - *Dispersivity – Determined through model calibration (if using a multi-dimensional model) by comparing model simulated contaminant dispersion with the spread of contaminant downgradient from source area. With simple analytical model, use methods of Xu and Eckstein (1995) for longitudinal dispersivity, Gelhar and others (1992) for transverse dispersivity, and use a very low vertical dispersivity as described in the in BIOSCREEN manual (Newell and others, 1996). Methods of estimating dispersivity that have been presented in Pickens and Grisak (1981), ASTM (1995), and USEPA (1986), appear to overstate the degree of contaminant dispersion and underestimate contaminant concentrations along the plume centerline.*

- *Organic carbon fraction – Determined through analysis for Total Organic Carbon (TOC) in soil or sediment samples. TOC should be analyzed in at least four soil or sediment samples per distinct layer.*
- *Octanol-carbon partition coefficient – Use a range of values provided in the literature [e.g. Howard and others, (1991)].*
- *Soil bulk density – Use a range of values provided in the literature.*
- *Decay rate – Determine through time-trend analysis of water quality analyses in representative monitoring wells (Newell and others, 2002). For this to be effective, it would need to be demonstrated that the contaminant plume has stabilized.*

- *Calibrate the model by comparing model simulated contaminant concentrations with field data at key monitoring wells.*

- *Present in table form, a sensitivity or uncertainty analysis, by adjusting the values of model input parameters and observing the impact on model predictions of contaminant concentrations at the compliance boundary.*

- *Present model predictions as range of possible outcomes given range of uncertainty in model input data. It is suggested to run the best and worst case scenarios and the one that best fits the facility data.*

- *Describe the performance monitoring network and sampling schedule to monitor remedy performance and to verify model predictions.*

How do the model predictions relate to an appropriate performance monitoring network for natural attenuation?

Model predictions may state that the plume has stabilized and that contaminant mass will be removed as a result of degradation. In this case, monitoring wells should be placed at appropriate locations to verify these predictions. The performance monitoring network should consist of an appropriate number of monitoring wells, preferably nested, along the centerline of the contaminant plume and around its perimeter. Model predictions may also state that contaminant concentrations will not exceed a cleanup criteria or facility specific target level at a downgradient location or receptor. In this case, monitoring wells should be placed at appropriate locations up gradient of the receptor to verify model predictions.

Is a performance monitoring network always necessary?

Yes, per Section 21309a(2)(c) “a monitoring plan if monitoring of environmental media or site activities or both is required to confirm the effectiveness and integrity of the remedy”, and Section 20118(10)a-c “an aquifer monitoring plan shall be part of all remedial action plans that address aquifer contamination.”

Appendix B.

Suggested References

The following references are grouped into general categories related to modeling. This list is intended to provide background information for staff so that they may develop a better understanding of different aspects of groundwater and fate-and-transport modeling. This reference list is not meant to be all inclusive.

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Appendix C.

Glossary of Modeling Terms

Absorption - dissolving or mixing of a substance in gaseous, liquid, or solid form with groundwater.

Adsorption - adherence of molecules in solution to the surface of solids.

Adsorption Isotherm - the graphical representation of the relationship between the solute concentration and the mass of the solute species adsorbed on the aquifer sediment or rock.

Advection - the process by which solutes are transported by moving groundwater. This is also called convective transport.

Analytical Element Model – a numerical procedure for modeling groundwater-flow that defines sources, sinks, and parameters as complex variables, called "analytic elements" that are solved together by the **Method of Superposition**.

Analytical Model - a mathematical model generally assuming homogeneous aquifer properties, uniform flow direction and hydraulic gradient, uniform aquifer thickness, with simple upper and lower boundaries, and lateral boundaries are placed at an infinite distance.

Anisotropy - the condition of having different values of a property (e.g. hydraulic conductivity) in different directions in geologic materials. This is especially apparent in fractured bedrock or layered sediment. Anisotropy is generally addressed in a model by aligning the major axis of the model grid along the principal directions of the anisotropy.

Aquifer - a geologic formation, group of formations, or part of a formation that is saturated, and is capable of providing a significant quantity of water.

Aquifer, Confined - an aquifer bounded above and below by confining beds in which the hydraulic-head is above the top of the aquifer.

Aquifer, Unconfined - an aquifer that has a hydraulic head surface (water table) which is in equilibrium with atmospheric pressure.

Area of Influence of a Well - the area surrounding a well over which the potentiometric surface has changed as the result of pumping groundwater from or recharging groundwater to an aquifer. Same as **Zone of Influence**. This is not to be confused with the **Capture Area of a Well**.

Base Flow - the part of stream flow that is attributable to long term discharge of groundwater to the stream. This part of stream flow is not attributable to short term surface run off, precipitation or snow melt events.

Biodegradation, Aerobic - decomposition of organic matter by microorganisms in the presence of free oxygen. The decomposition end-products include carbon dioxide and water.

Biodegradation, Anaerobic - decomposition of organic matter by microorganisms in the absence or near absence of free oxygen. Other electron acceptors than oxygen are used by bacteria in this decomposition process. The decomposition end-products are enriched in carbon.

Boundary Condition - a mathematical statement specifying the dependent variable (e.g. hydraulic head) at the boundaries of the modeled domain which contain the equations of the mathematical model. Examples are **Specified Head**, **Specified Flux**, or **Mixed Boundaries**.

Calibrated Model - a model for which all residuals between calibration targets and corresponding model outputs, or statistics computed from residuals, are less than pre-set acceptable values.

Calibration - the process of refining the model representation of the hydrogeologic framework, hydraulic properties, and boundary conditions to achieve a desired degree of correspondence between the model simulations and observations of the groundwater-flow system, which includes both measured hydraulic-head and flux.

Calibration Target - measured, observed, calculated, or estimated hydraulic-heads or groundwater-flow rates that a model must reproduce, at least approximately, to be considered calibrated.

Capillary Fringe - the basal region of the vadose zone comprising soil or sediments that are saturated, or nearly saturated, near the water table, gradually decreasing in water content with increasing elevation above the water table. The thickness of the capillary fringe is a function of the soil or sediment properties. Finer grained soil or sediment will have a greater capillary fringe thickness than coarse grained soil or sediment.

Cell - also called element, a distinct one- two- or three-dimensional model unit representing a discrete portion of a physical system with uniform properties assigned to it.

Computer Code (Computer Program) - the assembly of numerical techniques, bookkeeping, and control language that represents the model from acceptance of input data and instructions to delivery of output. Examples: MODFLOW, BIOSCREEN, MT3D, etc.

Concentration Gradient - the rate of change in solute concentration per unit distance at a given point and in a given direction.

Conceptualization Error - a modeling error where model formulation is based on incorrect or insufficient understanding of the modeled system.

Conceptual Site Model - an interpretation of the characteristics and dynamics of an aquifer system which is based on an examination of all available hydrogeological data for a modeled area. This includes the external configuration of the system, location and rates of recharge and discharge, location and hydraulic characteristics of natural boundaries, and the directions of groundwater-flow throughout the aquifer system.

Cone of Depression - a depression of the potentiometric surface that develops around a well that is being pumped.

Confining Bed (Confining Unit) - a hydrogeologic unit of less permeable material bounding one or more aquifers. Synonymous with **Aquitard, Aquiclude, and Aquifuge**.

Constant-Head Boundary - see **Specified Head Boundary**.

Constant-Head Node - a location in the discretized groundwater-flow model domain (node) where the hydraulic head remains the same over the time period considered; see also **Specified Head Boundary**.

Contaminant Fate - chemical changes and reactions that change the chemical nature of the contaminant.

Contaminant Transport Model - a model describing the movement of contaminants in the groundwater.

Contaminant Transport Velocity - the rate in which contamination moves through an aquifer.

Degradation Constant - term used to address the decay of contaminant concentration due to factors other than dispersion or diffusion.

Diffusion - process by which ions or molecules move in a random manner, because of their thermal kinetic energy, from areas of high solute concentrations to areas of low concentration in the direction of the solute concentration gradient. Also referred to as molecular diffusion.

Diffusion Coefficient - a constant of proportionality which relates the mass flux of a solute to the solute concentration gradient.

Discretization - the process of subdividing the continuous model and/or time domain into discrete segments or cells. Algebraic equations which approximate the governing flow and/or transport equations are applied to each segment or cell.

Dispersivity - a scale dependent property of an aquifer that determines the degree to which a dissolved constituent will spread in flowing groundwater. Dispersivity is comprised of three directional components - longitudinal, transverse, and vertical.

Dispersion - process by which some of the water molecules and solute molecules travel more rapidly than the average linear velocity and some travel more slowly due to the heterogeneity of hydraulic conductivity; spreading of the solute in the direction of the groundwater-flow (longitudinal dispersion) or direction perpendicular to groundwater-flow (transverse dispersion).

Dispersion Coefficient - (1) a measure of the spreading of a flowing substance due to the nature of the porous medium, with its interconnected channels distributed at random in all directions; (2) the sum of the coefficients of mechanical dispersion and molecular diffusion in a porous medium.

Distribution Coefficient - the quantity of the solute, chemical or radionuclide sorbed by the solid per unit weight of solid divided by the quantity dissolved in the water per unit volume of water.

Drawdown - the vertical distance the potentiometric surface is lowered due to the removal of water from a hydrogeologic unit.

Eh - also known as redox potential. Eh is a numerical measure of the intensity of oxidation or reducing conditions. A positive potential indicates oxidizing conditions and a negative potential indicates reducing conditions.

Elevation Head - that part of hydraulic-head which is attributable to the elevation of a measuring point (e.g. mid-point of a well screen) above a given datum (e.g. NAVD88).

Equipotential Line - a line connecting points of equal hydraulic head (potential). A set of such lines provides a contour map of a potentiometric surface.

Facility Characterization – For purposes of this document: (1) a general term applied to the investigation activities at a specific location that examines natural phenomena and human-induced conditions important to the resolution of environmental, safety and water resource issues; (2) means the program of exploration and research, both in the laboratory and in the field, undertaken to establish the geologic conditions and the ranges of those parameters of a particular facility relevant to the program. Facility characterization includes geophysical testing, borings, surface excavations, excavation of exploratory shafts, limited subsurface lateral excavations and borings and in situ testing at depth needed to determine the suitability of the facility.

Field Characterization - a review of historical, on- and off-site, as well as surface and sub-surface data and the collection of new data to meet project objectives; field characterization is a necessary prerequisite to the development of a conceptual site model.

Finite-Difference Method (FDM) - a discretization technique for solving a partial differential equation (PDE) by (1) replacing the continuous domain of interest by a finite number of regular-spaced mesh- or grid-points (i.e., nodes) representing volume-averaged sub-domain properties; and (2) by approximating the derivatives of the PDE for each of these points using finite differences; the resulting set of linear or nonlinear algebraic equations is solved using direct or iterative matrix-solving techniques.

Finite-Element Method (FEM) - similar to finite-difference method with the exception that (1) the mesh may consist of regular or irregular-spaced grid points which may have irregular shapes; and (2) the PDE is approximated using the method of weighted residuals to obtain a set of algebraic equations. These algebraic equations are solved using direct or iterative matrix-solving techniques.

Finite-Difference Model - a type of numerical model that uses a mathematical technique called the finite-difference method to obtain an approximate solution to the governing partial differential equation (in space and time).

Finite-Element Model - a numerical model that uses a mathematical technique called the finite-element method to obtain an approximate solution to the governing partial differential equation (in space and time).

Flow Path - the subsurface course a water molecule or solute WOULD follow in a given groundwater velocity field.

Flux - the volume of fluid or mass of a contaminant crossing a unit cross-sectional surface area per unit time.

Groundwater - that part of the subsurface water that is in the saturated zone.

Groundwater Basin - a groundwater system that has defined boundaries and may include more than one aquifer of permeable materials, which are capable of furnishing a significant water supply. Note - a basin is normally considered to include the surface area and the permeable materials beneath it. The surface-water divide need not coincide with a groundwater divide.

Groundwater Discharge - the water released from the zone of saturation; also the volume of water released.

Groundwater-Flow - the movement of water in the zone of saturation.

Groundwater-Flow Model - an application of a mathematical model to represent a regional or SITE-specific groundwater-flow system.

Groundwater-Flow System - a water saturated aggregate of aquifers and confining units in which water enters and moves and which is bounded by a basal confining unit that does not allow any vertical water movement and by zones of interaction with the earth's surface and with surface water systems. A groundwater-flow system has two basic hydraulic functions: it is a reservoir for water storage, and it serves as a conduit transmitting water from recharge to discharge areas. A groundwater-flow system may transport dissolved chemical constituents and heat.

Groundwater-Modeling Code - the computer code used in groundwater modeling to represent a non-unique, simplified mathematical description of the physical framework, geometry, active processes, and boundary conditions present in a reference subsurface hydrologic system.

Head (Total, Hydraulic-Head) - the height above a datum plane (such as sea level) of the column of water that can be supported by the hydraulic pressure at a given point in a groundwater system. In a well, it is the elevation of the height of water in a well above the mid-point of a well screen (**Pressure-Head**) plus the elevation of the mid-point of the well screen (**Elevation-Head**).

Head-Dependent Boundary – see **Mixed Boundary**.

Heterogeneity - a characteristic of a medium in which material properties vary spatially.

History-Matching – see **Model Verification**.

Homogeneity - a characteristic of a medium in which material properties are identical everywhere.

Hydraulic Conductivity - a constant of proportionality which relates the rate of groundwater-flow to the hydraulic-head gradient. It is a property of the porous media (**Intrinsic Permeability**) and the density and viscosity of the water moving through the porous media. It is defined as the volume of water at the existing kinematic viscosity that will move in a unit time under unit hydraulic gradient through a unit area measured at right angles to the direction of low. Estimated by, in order of preference, aquifer tests, slug tests, grain size analysis.

Hydraulic Gradient - the change in total hydraulic-head per unit distance of flow at a given point and in the direction of groundwater-flow.

Hydraulic-Head - the height above a datum plane (such as sea level) of the column of water that can be supported by the hydraulic pressure at a given point in a groundwater system. For a well, the hydraulic-head is equal to the distance between the water level in the well and the datum plane.

Hydraulic Properties - properties of soil and rock that govern the entrance of water and the capacity to hold, transmit and deliver water, e.g. porosity, effective porosity, specific retention, permeability and direction of maximum and minimum permeability.

Hydrologic Boundaries - physical boundaries of a hydrologic system.

Hydrologic Unit - geologic strata that can be distinguished on the basis of capacity to yield and transmit fluids. Aquifers and confining units are types of hydrologic units. Boundaries of a hydrologic unit may not necessarily correspond either laterally or vertically to lithostratigraphic formations.

Impermeable Boundary - the conceptual representation of a natural feature such as a fault or depositional contact that places a boundary of significantly less-permeable material laterally adjacent to an aquifer.

Intrinsic Permeability - a term describing the relative ease with which a porous medium can transmit a liquid under a hydraulic gradient or potential gradient. It is distinguished from hydraulic conductivity in that it is a property of the porous medium alone and is independent of the nature of the liquid or the potential field.

Inverse Method - a method of calibrating a groundwater-flow model using a computer code to systematically vary inputs or input parameters to minimize residuals or residual statistics.

Kriging - a geostatistical interpolation procedure for estimating spatial distributions of model inputs from scattered observations.

Leakage - (1) the flow of water from one hydrogeologic unit to another. The leakage may be natural, as through semi-impervious confining layer, or human made, as through an uncased well; (2) the natural loss of water from artificial structures as a result of hydrostatic pressure.

Leakance - (1) the ratio of the vertical hydraulic conductivity of a confining unit divided by its thickness; (2) the rate of flow across a unit (horizontal) area of a semi-pervious layer into (or out of) an aquifer under one unit of head difference across this layer. Synonymous with “coefficient of leakage”.

Leaky Aquifer - aquifers, whether artesian or water table, that lose or gain water through adjacent less permeable layers.

Mathematical Model – (1) a set of mathematical equations expressing the physical system and including simplifying assumptions; (2) the representation of a physical system by mathematical expressions from which the behavior of the system can be deduced with known accuracy.

Mixed Boundary – a linear combination of head and flux at a boundary. An example of a mixed boundary is leakage between a river and an underlying aquifer.

Model - an assembly of concepts in the form of mathematical equations that portray an understanding of a natural phenomenon.

Model Construction - the process of transforming the conceptual model into a mathematical model with hydraulic parameters. Model construction requires a-priori selection of a computer code.

Model Grid - system of connected nodal points superimposed over the problem domain to spatially discretize the problem domain into cells (finite-difference method) or elements (finite-element method) for the purpose of numerical modeling.

Modeling - the process of formulating a model of a system or process.

Model Input - the coefficients, system parameters, forcing terms, auxiliary conditions and program control parameters required to apply a computer code to a particular problem.

Modeling Objectives - the purpose(s) of a model application.

Model Verification - in model application: (1) the procedure of determining if a (facility-specific) model's accuracy and predictive capability lie within acceptable limits of error by tests independent of the calibration data; (2) in model application: using the set of parameter values and boundary conditions from a calibrated model to acceptably approximate a second set of field data measured under similar hydrologic conditions. Also referred to as **History-Matching**.

Node (Nodal Point) - in a numerical model, a location in the discretized model domain where a dependent variable (hydraulic head) is computed.

No-Flow Boundary - model boundary which is a **Specified-Flux Boundary** where the assigned flux is equal to zero. May correspond to a streamline or groundwater divide. Also see **Boundary Condition.**

Numerical Methods - in subsurface fluid flow modeling, a set of procedures used to solve the groundwater-flow equations in which the applicable partial differential equations are replaced by a set of algebraic equations written in terms of discrete values of dependent variables (e.g. hydraulic-head) at discrete points in space and time. The most commonly used numerical methods in groundwater-models are the finite-difference method, the finite-element method, the boundary-element method, and the analytic-element method.

Numerical Model - in subsurface fluid flow modeling, a mathematical model that uses numerical methods to solve the governing equations of the applicable problem.

Numerical Solution - an approximate solution of a governing (partial) differential equation derived by replacing the continuous governing equation with a set of equations in discrete points of the model's time and space domains.

Optimization – the process of determining the absolute or global minimum of an objective function (e.g. minimize head residual, maximize pumping rate, maximize hydraulic gradient magnitude, etc.) subject to appropriate constraints (e.g. bounds on values of independent parameters such as hydraulic conductivity, groundwater recharge rates, groundwater pumping rates, etc.). May apply to **Parameter Estimation Models** or Groundwater Management Models.

Parameter - any of a set of physical properties which determine the characteristics or behavior of a system.

Parameter Estimation Model (inverse model) - a computer code for determination of selected unknown parameters and stresses in a groundwater system, given that the response of the system to all stresses is known and that information is available regarding certain parameters and stresses.

Partitioning Function - a mathematical relation describing the distribution of a solute between solution and other phases.

Peclet Number - a relationship between the advective and diffusive components of solute transport expressed as the ratio of the product of the average interstitial velocity, times the characteristic length, divided by the coefficient of molecular diffusion; small values indicate diffusion is the dominant transport process, large values indicate advection dominance.

Perched Ground Water - unconfined groundwater separated from an underlying body of ground water by an unsaturated zone.

Percolation - the movement of water through the vadose zone, in contrast to infiltration at the land surface and recharge across the water table.

Piezometric Surface - see **Potentiometric Surface**

Porosity, Total - the ratio of the volume of void spaces in a rock or sediment to the total volume of the rock or sediment.

Porosity, Effective - (1) the ratio of the volume of the voids of a soil or rock mass that can be drained by gravity to the total volume of the mass; (2) the amount of interconnected pore space and fracture openings available for the transmission of fluids, expressed as the ratio of the volume of interconnected pores and openings to the volume of rock.

Post-Audit – the process of comparing model predictions against the field data or performance monitoring data to re-assess the accuracy of the conceptual model and model calibration.

Post-processing - using computer programs to analyze, display and store results of model simulations.

Potentiometric Surface - an imaginary surface representing the hydraulic-head of groundwater. The water table is a particular potentiometric surface. In cases where the head varies with depth in the aquifer, a potentiometric surface is meaningful only if it describes the hydraulic-head along a particular specified surface or stratum in that aquifer. More than one potentiometric surface is needed to describe the distribution of head in this case.

Pre-processing - using computer programs to assist in preparing data sets for use with generic simulation codes; may include grid generation, parameter allocation, control parameter selection, and data file formatting.

Pressure-Head - the head of water at a point in a porous system; negative for unsaturated systems, positive for saturated systems. Quantitatively, it is the water pressure divided by the specific weight of water.

Reaction Path Modeling - a simulation approach to studying the chemical evolution of a (natural) system.

Recharge, Groundwater - the process of water addition to the saturated zone usually from precipitation and percolation through the unsaturated zone to the water table.

Residual - the difference between the model-computed and field-measured values of a variable, such as hydraulic-head or groundwater-flow rate, at a specific time and location.

Retardation Factor - is used to simulate the resistance of the contamination to move through the groundwater aquifer due primarily to sorption of the contaminant to aquifer solids or entrapment of the contaminant in "dead-end" pores or fractures. A factor of one (1) represents the least resistance while increasing values show increasing resistance.

Saturated Zone - that part of the subsurface beneath the regional water table in which all voids, large and small, are filled with water under pressure greater than atmospheric.

Seepage Face - a physical boundary segment of a groundwater system along which groundwater discharges to ground surface and which is present when a water-table surface ends at the downstream external boundary of a flow domain; along this boundary segment, of which the location of the upper end is a-priori unknown, water pressure equals atmospheric pressure and hydraulic head equals elevation head. Commonly referred to as "seeps" or "springs".

Semi-Analytical Model - a mathematical model in which complex analytical solutions are evaluated using approximate techniques, resulting in a solution discrete in either the space or time domain.

Sensitivity - the variation in the value of one or more output variables (such as hydraulic heads) or quantities calculated from the output variables (such as groundwater-flow rates) due to changes in the value of one or more inputs to a groundwater-flow model (such as hydraulic properties or boundary conditions).

Sensitivity Analysis - a procedure based on systematic variation of model input values (1) to identify those model input elements that cause the most significant variations in model output; and (2) to quantitatively evaluate the impact of uncertainty in model input on the degree of calibration and on the model's predictive capability.

Simulation - in groundwater modeling, one complete execution of a groundwater modeling computer program, including input and output. Simulation is sometimes also used broadly to refer to the process of modeling in general.

Sink - in subsurface fluid flow modeling, a process whereby, or a feature from which, water is extracted from the groundwater-flow system.

Soil Bulk Density - the mass of dry soil per unit volume bulk soil.

Solubility - the total amount of solute that will remain indefinitely in a solution maintained at constant temperature and pressure in contact with the solid crystals from which the solutes were derived.

Solute-Transport Model - application of a model to represent the movement of chemical species dissolved in groundwater.

Sorption - (1) a general term used to encompass the process of absorption and adsorption; (2) all processes which remove solutes from the fluid phase and concentrate them on the solid phase of the medium.

Source - a process, or a feature, from which, water, vapor, NAPL, solute, or heat is added to the groundwater or vadose-zone flow system.

Source of Contaminants - the physical location (and spatial extent) of the source contaminating the aquifer; in order to model fate-and-transport of a contaminant, the characteristics of the contaminant source must be known or assumed.

Source Loading - the rate at which a contaminant is entering the groundwater system at a specific source.

Specific Capacity - the rate of discharge from a well divided by the drawdown of the water level within the well at a specific time since pumping started.

Specific Discharge - the rate of discharge of groundwater per unit area of a porous medium measured at perpendicular to the direction of groundwater-flow. Synonymous with flow velocity, darcian velocity, and specified flux.

Specific Storage - the volume of water released from, or taken into, storage per unit volume of the porous medium per unit change in head.

Specific Yield - the ratio of the volume of water that the saturated rock or soil will yield by gravity to the volume of the rock or soil. In the field, specific yield is generally determined by tests of unconfined aquifers and represents the change that occurs in the volume of water in storage per unit area of unconfined aquifer as the result of a unit change in head. Such a change in storage is produced by draining or filling of pore space and is, therefore, mainly dependent on particle size, rate of change of the water table, and time of drainage.

Specified-Flux Boundary - model boundary condition in which the groundwater flux is specified; also called fixed or prescribed flux, or Neumann boundary condition.

Specified-Head Boundary (Constant Head) - a model boundary at which the hydraulic head is specified; also called fixed or prescribed head, or Dirichlet boundary condition.

Steady-State Conditions - a condition in which system inputs and outputs are in equilibrium so that there is no net change in the system with time.

Steady-State Flow - a characteristic of a groundwater or vadose-zone flow system where the magnitude and direction of specific discharge at any point in space are constant in time.

Storage Coefficient - the volume of water an aquifer releases from or takes into storage per unit surface area of the aquifer per unit change in head. For a confined aquifer, the storage coefficient is equal to the product of the specific storage and aquifer thickness. For an unconfined aquifer, the storage coefficient is approximately equal to specific yield.

Storativity - see **Storage Coefficient**.

Superposition Principle - the addition or subtraction of two or more different solutions of a governing linear partial differential equation (PDE) to obtain a compoSITE solution of the PDE. As an example, the superposition of drawdown caused by a pumping well on a regional , non-pumping potentiometric surface.

Transient Conditions - a condition in which system inputs and outputs are not in equilibrium so that there is a net change in the system with time.

Transient Flow - a condition that occurs when, at any location in a groundwater or vadose-zone flow system, the magnitude and/or direction of the specific discharge changes with time.

Transmissivity - the volume of water at the existing kinetic viscosity that will move in a unit time under a unit hydraulic gradient through a unit width of the aquifer. It is the product of the hydraulic conductivity multiplied by the aquifer thickness.

Unsaturated Zone - the zone between the land surface and the water table that may include the capillary fringe. Water in this zone is generally under less than atmospheric pressure and some of the voids may contain air or other gases at atmospheric pressure. Beneath flooded areas or in perched water bodies the water pressure locally may be greater than atmospheric.

Vadose zone - see **Unsaturated Zone**.

Vadose zone Flow System - an aggregate of rock, in which both water and air enters and moves and which is bounded by rock that does not allow any water movement, and by zones of interaction with the earth's surface, atmosphere and surface water systems. A vadose zone flow system has two basic hydraulic functions: it is a reservoir for water storage and it serves as a conduit by facilitating the transmission of water from intake to discharge areas, integrating various inputs and dampening and delaying the propagation of responses to those inputs. A vadose zone flow system may transport dissolved chemical constituents and heat.

Velocity, Darcian - See **Specific Discharge**.

Velocity, Average Interstitial - the average rate of groundwater-flow to interstices expressed as the product of hydraulic conductivity and hydraulic gradient divided by the effective porosity. Synonymous with average linear groundwater velocity, or effective velocity.

Water Mass Balance - an inventory of the different sources and sinks of water in a hydrogeologic system. In a well-posed model, the sources and sinks should balance.

Water Table - the surface of a groundwater body at which the water pressure equals atmospheric pressure. Earth material below the water table is saturated with water.

Zone of Saturation - a hydrologic zone in which all the interstices between particles of geologic material or all of the joints, fractures, or solution channels in a consolidated rock unit are filled with water under pressure greater than that of the atmosphere.

Appendix D.

Suggested Groundwater Model Documentation Report Format

Recommended Format for Model Documentation Report

- ✓ *Problem Statement and Model Application Goals* - Provide a brief description of the problem(s) to be addressed and the purpose and goal of the model application.
- ✓ *Hydrogeologic Characterization* - Provide a detailed description, in text, tables and figures, of the hydrogeologic framework, hydrologic boundaries, hydraulic properties, hydraulic-head distribution and hydraulic stresses of the modeled area. Processes for determining hydraulic properties should be described in detail.
- ✓ *Contaminant* Characterization - Provide a detailed description, in text, tables and figures, of the nature (identified chemicals and media-type that are impacted) and horizontal and vertical extent of contaminants in the modeled area.
- ✓ *Identification of Migration Pathways* - Describe the migration of the chemicals of concern from the source area to the downgradient delineated extent of contamination. Also describe possible migration pathways beyond the extent of contamination.
- ✓ *Describe the Fate-and-transport Processes* – Describe, in detail, the attenuation processes that impact contaminant concentrations.
- ✓ *Identify Impacted or Potentially-Impacted Receptors* – All impacted receptors, or those that have the potential to be impacted, need to be identified.
- ✓ *Model Conceptualization* - Provide a description of the representation of hydrogeologic and/or geochemical and contaminant conditions in the facility model. Identify the source of all the input used in the modeling, whether derived from published sources or measured or calculated from field or laboratory testing. Discuss the processes by which the calculated input parameters were generated.
- ✓ *Modeling Software Selection* - Identify the model selected [type (e.g. analytical fate-and-transport) and software (e.g. BIOSCREEN)], its version number, and describe its applicability and limitations as they relate to the problem to be simulated. The model should be capable of simulating the hydraulic, geochemical and contaminant conditions at the facility.
- ✓ *Model Calibration* - Describe the process by which model input parameters were selected to achieve a match between model-simulated conditions and field conditions and describe, in text tables and figures, the degree to which modeled conditions match actual field conditions.
- ✓ *History matching (model verification)* – If appropriate, perform additional simulations using the calibrated model to ensure that it is capable of reproducing a different set of historical facility conditions. Discuss the results of these simulations.
- ✓ *Sensitivity or Uncertainty Analysis* - Report in text, tables and figures the results of a model sensitivity analysis that varies all appropriate model input parameters over a realistic range that reflects the uncertainty in the value of that parameter.

- ✓ *Predictive Simulations or Use of Model for Evaluation of Remedial Alternatives* - Present all model predictive or remedial alternative simulations as a range of probable results given the range of uncertainty in model parameters.
- ✓ *Recommendations and Conclusions*.
- ✓ *References* – Provide references for all reports cited in the model documentation report.
- ✓ *Appendices* – Provide data, reports, correspondence, or work plans used in support of the model that are not included in the body of the model documentation report.

Tables

The following are examples of information that may be presented in table format:

- ✓ Well construction details.
- ✓ Elevation data.
- ✓ Static, or transient, water-level elevation data.
- ✓ Hydraulic conductivity or transmissivity test results.
- ✓ Groundwater quality analyses.
- ✓ Model calibration and verification results showing a comparison of measured and simulated calibration targets and residuals.
- ✓ Results of sensitivity analyses showing the range of adjusted model parameters and resulting change in hydraulic heads or groundwater-flow rates.

Other data, not listed above, may lend itself to presentation in table format. Where appropriate, the aquifer for which the data apply should be clearly shown in each table.

Figures

All figures presented in the report should be drawn to the same scale. That is, all maps, whether they are for model input data, or model simulation results, should be drawn using the same map scale. This also holds for all cross sections. The following examples are figures that should be provided in the model documentation report:

- ✓ Regional location map with topography.
- ✓ Accurately scaled facility map showing soil boring and well locations, facility topography, and other pertinent features.
- ✓ Geologic cross sections.
- ✓ Iso-contour maps showing the measured and simulated hydraulic-head distribution.
- ✓ Iso-contour maps of top and/or bottom elevations of aquifers and confining units.
- ✓ Area-wide distribution of hydraulic conductivity/transmissivity.
- ✓ Map of area-wide recharge (if appropriate).
- ✓ Model grid with locations of different boundary conditions used in the model.

- ✓ Iso-contour maps of actual and simulated contaminant distribution and/or cross sections showing vertical distribution of contaminants (if appropriate).

Other types of information, not listed above, may be presented in graphic format. Figures that are used to illustrate derived or interpreted surfaces such as layer bottom elevations and hydraulic head maps should have the data used for the interpolation also posted on the figures. As an example, measured hydraulic-head maps should identify the observation points and the measured hydraulic-head elevation. Similarly, the simulated hydraulic-head maps should locate the calibration target points and the residual between the measured and modeled data.

Additional Data or Information

Additional data may be necessary in the model documentation report. Examples of additional data are as follows:

- ✓ Additional study work plans providing for the collection of additional data where model simulations show data deficiencies, and
- ✓ Groundwater monitoring plans/proposals/recommendations to collect data needed to verify model predictions.

Other data may be necessary, depending on the conditions at the facility. These additional subjects should be reflected within the body of the report. This may include additional figures, tables, or report sections.

Model Input Files

Model datasets in digital format will need to be provided as part of the model documentation if the model is to be reviewed. The datasets for the different simulations (model calibration, history matching and predictive simulations) need to be provided in digital format. Groundwater model input files will follow a format determined by the model software used by the model developer. In addition, the model input files may be compressed using software such as WinZip® in an attempt to store all data on a CD-ROM or DVD. As with other data submittals, it is necessary to prepare a MODEL_FILES.TXT file which describes the content of each model input file on the CD-ROM and the model software used to create the model data sets.

If a computer program is used that is proprietary and not currently supported by the Groundwater Modeling Program in the RRD, it may be necessary for the modeler to provide a copy of the model software for model review purposes only. The copy of this model software will be returned after model review has been completed. The Groundwater Modeling Program maintains current licenses of Groundwater Vistas©, Visual MODFLOW©, and GMS© software. Current copies of all commonly-used public domain software are also maintained. Please contact the GMP if this is an issue.

Appendix E.

References for Commonly Used Groundwater Modeling Software

This list provides references for the groundwater modeling software that are commonly used for applications in Michigan. References for modeling software that has not been used, or used very infrequently, are not included in this list. In the future, this list will be modified to reflect usage by the hydrogeologic modeling community.

BIOCHLOR

Aziz, C.E., C.J. Newell, J.R. Gonzales, P. Haas, T.P. Clement, and Y-W. Sun, 2000. BIOCHLOR: Natural Attenuation Decision Support System User's Manual Version 1.0. EPA/600/R-00/008. U.S. Environmental Protection Agency, Ada, OK.

Aziz, C.E., C.J. Newell, and J.R. Gonzales, 2002. BIOCHLOR: Natural Attenuation Decision Support System Version 2.2 Users Manual Addendum.

BIOSCREEN

Newell, C.J., J. Gonzales, and R. McLeod, 1996. BIOSCREEN Natural Attenuation Decision Support System. EPA/600/R-96/087. U.S. Environmental Protection Agency, Ada, OK.

BIOSCREEN-AT

Karanovic, M., C.J. Neville, and C.B. Andrews, 2007. BIOSCREEN_AT: BIOSCREEN with an Exact Analytical Solution. Ground Water, Vol. 45, No. 2, pp. 242-245.

BIOPLUME II

Rifai, H.S., P.B. Bedient, R.C. Borden, and F.F. Haasbeek, 1988. BIOPLUME II – Computer Model of Two-Dimensional Transport under the Influence of Oxygen Limited Biodegradation in Ground Water. EPA/600/8-88/093a. U.S. Environmental Protection Agency, Ada OK.

BIOPLUME III

Rifai, H.S., C.J. Newell, J.R. Gonzales, S. Dendrou, B. Dendrou, L. Kennedy, and J.T. Wilson, 1998. BIOPLUME III: Natural Attenuation Decision Support System User's Manual Version 1.0. EPA/600/R-98/010. U.S. Environmental Protection Agency, Ada OK.

MOC

Konikow, L.F., and J.D. Bredehoeft, 1978. Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water. U.S. Geological Survey Water-Resources Investigations Book 7, Chapter C2, 90 p.

MODFLOW-88

McDonald, M.G., and A.W. Harbaugh, 1988. A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model. U.S. Geological Survey Techniques of Water Resources Investigations, Book 6, 586 p.

MODFLOW-96

Harbaugh, A.W., and McDonald, M.G., 1996, User's documentation for MODFLOW-96, an update to the U.S. Geological Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 96-485, 56 p.

Harbaugh, A.W., and McDonald, M.G., 1996, Programmer's documentation for MODFLOW-96, an update to the U.S. Geological Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 96-486, 220 p

MODFLOW-2000

Harbaugh, A.W., Banta, E.R., Hill, M.C., and McDonald, M.G., 2000, MODFLOW-2000, the U.S. Geological Survey modular ground-water model -- User Guide to Modularization Concepts and the Ground-Water Flow Process: U.S. Geological Survey Open-File Report 00-92, 121 p.

Hill, M.C., Banta, E.R., Harbaugh, A.W., and Anderman, E.R., 2000, MODFLOW-2000, the U.S. Geological Survey modular ground-water model -- User Guide to the Observation, Sensitivity, and Parameter-Estimation Processes and Three Post-Processing Programs: U.S. Geological Survey Open-File Report 00-184, 210 p.

MODFLOWP

Hill, M.C., 1992. A Computer Program (MODFLOWP) for Estimating Parameters of a Transient, Three-Dimensional Groundwater Flow Model Using Nonlinear Regression. U.S. Geological Survey Open File Report 91-484, 358 p.

MODPATH

Pollock, D.W., 1989. Documentation of Computer Programs to Compute and Display Pathlines Using Results from the U.S. Geological Survey Modular Three-Dimensional Finite-Difference Ground-Water Model. U.S. Geological Survey Open-File Report 89-381.

MT3D

Zheng, C., 1990. MT3D: a Modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems. Report to the U.S. Environmental Protection Agency, Ada, OK, 170 p.

PATH3D

Zheng, C., 1991. PATH3D, A Ground-Water Path and Travel-Time Simulator, User’s Manual, S.S. Papadopulos & Associates, Inc. Bethesda, MD.

PEST

Doherty, J., 2002. PEST: Model Independent Parameter Estimation, User's Manual, 5th edition. Watermark Numerical Computing.

RT3D

T.P. Clement, 1997. RT3D: A Modular Computer Code for Simulating Reactive Multi-Species Transport in 3-Dimensional Groundwater Systems. Pacific Northwest National Laboratory report PNNL-SA-11720. Version 1.0, 59 p.

T.P. Clement, and C. Johnson, 2002. RT3D Version 2.5 Update Document, 20 p.

UCODE

Poeter, E.P., and M.C. Hill, 1998. Documentation of UCODE, A Computer Code for Universal Inverse Modeling. U.S. Geological Survey Water-Resources Investigations Report 98-4080, 116 p.