COMMONWEALTH OF MASSACHUSETTS

DEPARTMENT OF ENVIRONMENTAL PROTECTION

STANDARD REFERENCES FOR MONITORING WELLS

SECTION 7.0 GROUNDWATER MODELING

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7.1 GROUNDWATER MODELING OVERVIEW

7.1-1 Introduction

Groundwater flow/solute transport models are tools designed to provide the user with greater understanding of, and the ability to quantify, groundwater flow and solute transport in an aquifer system. Groundwater models have been used for many years to simulate groundwater flow and are the basis for predicting solute transport in aquifers. The goal of groundwater modeling is to integrate the existing knowledge about an aquifer system such that it tests the conceptual model of the system (i.e., hypothesis testing). This is accomplished by predicting the value of an unknown variable (e.g., piezometric head or solute concentration at various points in an aquifer) given a specified set of initial and boundary conditions. Models are also used to determine flow to wells, flow to and from streams, heat transport in groundwater, regional flow patterns, flownet analyses, and production well design (Walton, 1985).

Mathematical models have gained wide acceptance in the groundwater field. This Standard Reference describes the basic differences between analytical and numerical models, outlines the principal steps in the construction of numerical groundwater flow and solute transport models, and provides recommended quality control procedures for modeling.

This section of the Standard References has been prepared in response to numerous requests for inclusion of some material about groundwater modeling. It represents an attempt by DEP to provide an overview of the subject. It does not represent an endorsement by DEP of any particular type of approach, but will discuss the appropriateness of using (or not using) a numerical rather than an analytical model in reports submitted to the department. It is outside the scope of this section to undertake an in-depth discussion of modeling techniques. Good documentation is a critical and often overlooked element in modeling. It is essential that, throughout the entire process, the modeler documents all steps performed, from the initial conceptual model through the various simulations to the final product.

7.1-2 Purpose

The purpose of a groundwater flow model is to be able to make predictions or gain insight into an aquifer system by creating, via mathematical expressions and equations, a simulation of the distribution of piezometric head in an aquifer. This simulated data set of piezometric heads represents values that have been measured at specific locations (i.e., monitoring wells, piezometers, staff gages). Once a model has been created and properly calibrated (i.e., a process of comparing simulated vs. measured heads and adjusting the model parameters accordingly), the model can be used to forecast what the distribution of head might be for a different set of pumping, recharge or aquifer conditions.

7.1.3 General Applications

There are many applications for groundwater flow models. It might be important, for example, to know what the resulting water table might look like if a cutoff wall or french drain were installed in the aquifer, or what the influence of a lagoon or impoundment would have on the flow field, or what the capture zone of a recovery well might be for different pumping rates. Larger scale applications include defining a well head protection area for a municipal water supply or predicting the geometry of a contaminant plume.
One word of caution is offered to the reader: models do not necessarily provide unique solutions when groundwater flow or contaminant transport are being modeled, since combinations of different hydrogeologic and contaminant transport parameters can produce similar results. Groundwater modeling is not an easy task. At a minimum, an in-depth understanding of groundwater flow is required. A reliable model begins with collection of comprehensive data on the aquifer being studied and ends with calibration to a wide distribution of known heads. Care must be taken not to misuse models, which may lead to erroneous conclusions. Misuse of models is more likely to occur if the data base on the aquifer is limited and does not contain significant information with which to compare and verify the response of the model.

In addition, on a larger site, as new field data is acquired, the model can be periodically updated. Thus a "second", or even "third", generation model may be constructed as more monitoring wells are installed, or as the boundary conditions are better understood, or as more water quality information is gathered.

7.2 MODELING TERMINOLOGY

7.2-1 Terminology

There are a few basic terms that must be understood in order to discuss groundwater models:

Advection - Advection is the transport of a non-reactive or conservative solute (i.e., a solute that travels without undergoing reactions with the aquifer matrix) at the average groundwater velocity that is equal, in a homogeneous porous media, to the specific discharge (q) divided by the porosity (n).

Boundary Conditions - Boundary conditions are site-specific physical or hydraulic conditions that describe the flux or piezometric head conditions at the edges of the groundwater system. Physical boundaries are formed by the presence of an impermeable body of rock or significantly lower permeability unit or large body of water while hydraulic boundaries include groundwater divides and streamlines. These boundaries, described as mathematical expressions in the model, have a dominant effect on defining groundwater flow in the aquifer being modeled. Poorly defined boundary conditions will result in a problem that is ill defined and for which no meaningful solution can be obtained. There are three basic types of boundary conditions that are used in constructing numerical flow models:

1. Specified head - The piezometric head is known for surfaces bounding the flow region. Examples include ponds, streams and reservoirs with an unchanging head that is in good hydraulic connection with the aquifer or an equipotential line of known value. As constant heads represent potentially infinite sources or sinks in the model, specification of such boundaries needs to be undertaken with care.

2. Specified flux - The flow rate (i.e., flux) is known across surfaces bounding the region. A leaky till/stratified drift boundary is an example of a specified-flow boundary. A special type of specified flux boundary is a no-flow boundary (an impervious or barrier boundary). Another example of a no-flow boundary is a groundwater divide or a flow line.

   Note: Equipotential lines or flow lines may be used as model boundaries as long as they are far enough away from nodes where pumping or recharging centers are located so that the boundaries are not influenced by these stresses.

3. Head-dependent flux - The flux is a function of head at this boundary. This is referred to as a mixed boundary because it relates boundary flux to boundary head. Its most common use is to represent interaction between a water table aquifer and a stream or river that is separated from the aquifer by a semi-pervious boundary (e.g., a silt bed lining the bottom of a channel).

Dispersion - Dispersion is the process of solute spreading and dilution as advection carries it along. It is the result of mechanical mixing as well as molecular diffusion that occurs as water migrates through a porous medium. In more permeable formation (i.e., sands and gravel) mechanical mixing and advection are the dominant processes by which a solute spreads from a source area. In low permeability formations such as clay or silty clay, molecular diffusion is generally the dominant process by which a solute migrates from a source area. It should be noted that if preferential migration pathways are present in the low permeability material, due to localized lithologic variations or the presence of vertical cracks, then advection and mechanicla mixing can play a dominant role as well.

Initial Conditions - Initial conditions are those conditions that exist in the aquifer at time equals zero in the simulation. For example, the elevation of the water table or piezometric head is often specified as an initial condition in transient groundwater flow models or initial concentrations would be specified in the case of a transient solute transport mode. In steady state simulations, the initial conditions may be relatively unimportant, but for transient simulations, the initial conditions are critical.

Model Calibration - Model calibration is the process of comparing computed values (e.g., piezometric head, stream base flow, etc.) that are determined at the end of a model run with actual values of head (i.e., measured in the field) and making adjustments to the nodal parameters or model boundary conditions until there is agreement between the two values. This is not a node-by-node exercise, but generally parameter values are varied over areas of the model to improve overall matching. While heads should match reasonably well, flow directions, hydraulic gradients and overall water balances may be even more important aspects of the calibration matching.

Model Construction - Model construction is the process of using the physical and hydrogeologic data obtained about the aquifer together with the modeler's conceptual model of the system and, by means of employing a model grid, assigning values such as hydraulic conductivity, transmissivity and storativity to each node. The boundary conditions and initial conditions are also specified during model construction as required by the conceptual model.

Model Grid - The model grid is a two or three-dimensional representation of the aquifer geometry. The model grid consists of connected quadrilaterals or triangles that resemble a screen mesh. Figure 7-1 depicts an aquifer and examples of what some two dimensional model grids might look like for finite difference or finite element model applications.

Model Simulation - A model simulation refers to the computer generating a set of piezometric heads.

Model Verification - Model verification is performed once the model is calibrated. The procedure for verifying a model is accomplished by running the model for a different set of conditions, and correspondingly a different set of measured heads, than the set that was used to calibrate the model. If the model is able to compute a set of heads for the second set of conditions that matches the field measured heads for those conditions, then the model is considered to be "verified" and "well calibrated". Care should still be exercised, however, when running the model under conditions much different than observed or calibrated.

Node - A node represents the physical position in the aquifer where the average hydrogeologic properties are defined and piezometric heads are calculated. In some models, the nodes are the centers of the grids (see Figure 7-1(b)) while in others they are the intersections of the grids (see Figure 7-1(c) and (d)). In a block centered grid, aquifer properties and hydraulic stresses are typically assigned to the block surrounding the node. In a mesh centered grid, properties are assigned to the area surrounding the node. Infinite element models, aquifer properties can either be assigned to the node or the element (Anderson and Woessner, 1992). The head at the node represents the average head for the area immediately adjacent to the node.

Solute Transport - Solute transport in groundwater is the migration of compounds in solution through a saturated, porous medium. Processes such as advection and dispersion are two of the dominant mechanisms that govern this process. A contaminant may be subject to other mechanisms such as retardation, chemical or biologic transformation, or volatilization that will reduce anticipated concentrations. A solute that does not degrade is said to be conservative.

Steady State - Steady state refers to an equilibrium condition whereby over long periods of time, hydrogeologic systems may achieve or approximate some non-changing conditions in which heads or concentrations do not change with further passage of time. Such systems are said to have achieved steady state. Models may deal with this in different ways. Some have "steady state" options, while others require the user to specify some long period of time and/or closure criterion beyond which changes in head are considered inconsequential.

Transient - Transient refers to a non-equilibrium condition whereby a model is allowed to run for a specified period of simulated time. Typically, initial conditions are steady state in order to correctly interpret head changes under transient conditions, due to stresses in the model, e.g., pumping.

7.3 MATHEMATICAL MODELS

While the earlier subsections of Section 7.3 are written primarily referencing flow modeling, the techniques and concepts apply equally to solute transport models. Section 7.3-4 discusses added considerations specific to solute transport.

7.3-1 Types of Models

A mathematical model is a set of equations that describes the physics of a system or process. Mathematical groundwater flow models are powerful tools for studying cause-and-effect relationships within groundwater systems. However, unlike physical or analog models, mathematical models provide varying degrees of tangible representation of the system that is being simulated. The types of mathematical models are stochastic or deterministic while solution techniques may be analytical or numerical.

Application of a stochastic model attempts to recognize that parameters do not have a single value over the domain of the aquifer. Instead, a parameter is likely to have a certain probability distribution, even for a relatively homogeneous material. Stochastic models attempt to account for this variance in the basic parameters by determining or assuming a probability distribution function (pdf) for some model input parameters. For example, hydraulic conductivity generally has a log-normal distribution, while other parameters may have normal distributions. The stochastic model (for example, the Monte Carlo method) randomly samples from the input parameter distribution and calculates a result. After a large number of iterations, possibly hundreds, enough data points are accumulated to identify a probability distribution for the output parameter. Initial data requirements can be large (to adequately determine the input variable distributions) and computer run time can be high (to provide the number of runs required to determine the output pdf). Stochastic models are rarely used except for very simple flow model situations.

Analytical models are equations that are the closed form solutions to the governing equations for flow and transport with appropriate boundary and initial conditions. In order to obtain the closed form solution, it is often necessary to assume a simplified aquifer condition, simple boundary conditions, and single values (no spatial distribution) for the input parameters. Depending on the situation, an analytical model may or may not be a good choice for accurately determining output parameter values for a specific site. However, it may be possible to select conservative values for the parameters and construct a worst-case scenario. If this approach provides satisfactory results, more detailed (i.e., numerical) modeling may not be necessary. Analytical models are generally used for simple systems and for screening types of analyses.

Numerical models employ a variety of numerical approximation methods to represent the partial differential equations that govern flow and transport. These include finite difference methods that use algebraic approximations, finite element methods that use minimization of residuals of weighting functions integrated over the model domain (Galerkin method), or approximations of equation forms over typical conditions of groundwater flow, such as the method of characteristics. Examples of numerical models using these various approaches are MODFLOW, AQUIFEM, and MOC, respectively. These approximations are applied over each model element or node, giving rise to a set of simultaneous equations that may then be either directly solved by matrix inversion methods, or, more typically, by iterative procedures that are more efficient than the matrix methods when large arrays are involved. Data requirements and levels of effort are generally much greater for numerical models than for analytical models.

The basic difference between analytical and numerical models is the degree of simplification that is assumed for the boundary conditions and physical system being modeled. The choice between selecting an analytical model or a numerical model may be a function of the goals of the modeling, available time and budget, and the quantity and quality of data for the site. Some modelers, however, will construct preliminary models with very little data and use the model as an aid to developing the field program. Often an analytical model, calculated for limiting (maximum or minimum expected) values of parameters, may provide a satisfactory basis for a decision (e.g., quantifying the volumetric rate of flow of groundwater into a recovery trench), and thus save the considerable expense and time required for a numerical model. In any case, a good conceptualization of the aquifer system is required in order to evaluate the applicability of any given model, and to appropriately include consideration of the underlying assumptions of that model.

7.3-2 Analytical Models

Analytical models frequently assume a substantial simplification of the groundwater system, but they provide exact solutions to the mathematical expression. In analytical models, the flow is most often described as occurring in confined aquifers that are assumed to be:

- homogeneous and isotropic;
- infinite in areal extent;
- uniform thickness throughout;
- groundwater temperature, density, and viscosity are assumed to be constant;
- production and injection wells have infinitesimal diameters and no storage capacity or finite diameters with specified storage capacity;
- except for flowing wells, areal discharge and recharge to the aquifer are constant (and might not be included); and
- hydrogeologic boundaries usually are not addressed in the general solution. However, boundary problems may be handled by using image well theory (Walton, 1985).

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Darcy's law, one form of which is given by the expression:

$$q = KJ$$

where:
q = specific discharge;
K = hydraulic conductivity; and
J = hydraulic gradient

is an equation of motion that reflects the most simple analytical model. Using it requires satisfying all of the conditions previously stated. If the hydraulic conductivity and hydraulic gradient are known, then the specific discharge can be quantified. Furthermore, given any two of the three parameters, the third variable can be calculated at any other location in an aquifer that has homogeneous, isotropic properties.

Other examples of analytical models include the Dupuit-Forcheimer discharge formula for flow in unconfined aquifers and Jacob's approximation of the Theis equation for predicting the transient drawdown response due to the influence of a pumping well. Some texts containing these and other analytical models include: "Hydraulics of Groundwater" (Bear, 1979), "Quantitative Hydrogeology" (deMarsily, 1986).

7.3-3 Numerical Models

Numerical models represent the equation of motion and statement of mass conservation of groundwater in an aquifer system. They rely on the same principles and equations as analytical models, but they generally require fewer simplifying assumptions. The theoretical basis for the governing groundwater flow equations is well documented and is based on a combination of Darcy's Law and the groundwater mass balance equation (Wang and Anderson, 1982; Mercer and Faust, 1981). Some of the principle input parameters necessary to construct a groundwater flow model at a specific site must be identified. These parameters include:

- the shape of the potentiometric surface for confined aquifers or the piezometric surface (i.e., the water table) for unconfined aquifers;

- the distribution of hydraulic conductivity, and depth to bedrock or transmissivity in the aquifer;

- the geometry of the aquifer; and
- the location and nature of recharge or barrier boundaries.

The potentiometric head (needed for model calibration) can be measured at selected locations in the field; transmissivity or hydraulic conductivity and depth to bedrock can be estimated with reasonable reliability using pumping or, if necessary, slug test data, boring log information, or a host of other field or lab tests (see Section 7.4-4.2 for greater elaboration); and the aquifer/aquitard geometry can be determined from boring log and pumping test information, surface geophysics and survey data. Geophysical techniques such as seismic refraction, electrical resistivity and ground penetrating radar are cost effective ways of characterizing aquifer geometry, stratigraphy and, to some degree, the depth to the water table.

The acquisition of this physical data, in conjunction with water quality results, is invariably limited in extent, principally because of economic considerations. It is, however, the primary and fundamental source of information upon which the model is constructed. Consequently, the inherent weakness associated with many modeling efforts is lack of sufficient data of usable quality. It behooves the project manager and modeler to continually be aware of this when conceptualizing and constructing models. It is also why the calibration procedure and sensitivity analysis are such an important part of the modeling process.

The discharge/recharge relationship of surface bodies of water (i.e., lakes, ponds and streams) within and adjacent to the aquifer needs to be identified in order to properly construct and calibrate the model. This data can be obtained by taking contemporaneous stream flow measurements at different locations in a stream or river during extended periods of little or no rainfall (three or four days) or by utilizing streamflow measurements at USGS gauging stations. The water that is in the stream channel during these times is referred to as base flow and represents almost entirely the groundwater portion of stream flow. Using a technique referred to as stream tube or flow net analysis, this information coupled with piezometric head data in the aquifer can be used to estimate the hydraulic conductivity in other parts of the aquifer. At the very least, this information will be needed to calibrate the model when the nodal water mass balance (i.e., the amount of water coming in and out of each node) is performed. Seepage meters may also be used to quantify flux between the aquifer and a surface water body. When used with piezometers below the streambed, hydraulic conductivity of the streambed can be estimated (Lee, 1978).

Gathering physical and chemical data for an aquifer is generally very costly and time consuming given:

- the geologic variability that exists in glaciated terrains such as New England; and
- the types and required detection limits of the contaminants that are being regulated.

That is why it is very important that the project manager, field geologist and modeler all have a good conceptual understanding of the hydrogeology of the aquifer. If the team lacks or is weak in any of these areas:

- a firm theoretical understanding of flow through a porous or fractured bedrock medium;
- the nature and characteristics of the contaminants in question;
- the influence that any production wells may have on regional flow;
- how the aquifer is bounded; and
- appropriate protocols for installing and sampling monitoring wells and conducting other field activities,

then the following will occur:

- a poorly defined conceptual model;
- the design and execution of an inadequate field sampling program;
- insufficient and/or inaccurate data with which to construct and calibrate a groundwater flow and, if appropriate, a solute transport model; and
- a poorly designed remedial strategy.

In most numerical models, the governing partial differential equations are approximated by algebraic difference expressions relating unknown variables (e.g., head, flux) at discrete points (nodes) at different times (Javandel et al., 1984). Consequently, more complex conditions such as heterogeneity and anisotropy can be more accurately simulated in numerical models than in analytical models. Typically, numerical models utilize more data than analytical models because varying aquifer properties may be described at numerous, discrete points within an aquifer. Complex or irregularly shaped boundaries such as leaky streams or impervious (i.e., no-flow) boundaries or a meandering river are generally easier to model using a numerical approach, while analytical models are severely constrained in this regard.

7.3-3.1 Finite-difference Technique

There are two common types of numerical techniques that are applied to groundwater problems: finite-difference and finite-element methods. Finite difference techniques solve the groundwater-flow equation by approximating the derivatives of partial differential equations at regularly or variably spaced points in the system. The finite-difference technique employs a grid of squares or rectangles as depicted in Figures 7-1(b) and (c). Figure 7-1(b) is a block centered representation of the aquifer shown in Figure 7-1(a), while Figure 7-1(c) is a mesh or node centered grid of the same aquifer. There is no significant difference between the two. If there are lateral variations in hydraulic properties within the aquifer, such as transmissivity or storativity that are linear in nature, use of a block centered grid makes it slightly easier to delineate and assign values to those regions.

Notice that in either case, (b) or (c), because of the perpendicular nature of the intersecting grid lines, some of the grid is either outside or inside the physical aquifer boundary. Since aquifer geometry and boundaries are rarely linear features, this condition will invariably arise. The only time that it may present a problem is if accurate piezometric data are desired adjacent to those features. If that is the case, then a finer grid size will result in a more accurate determination of piezometer head. However, a finer mesh will increase the number of nodes necessary to describe the feature, which in turn will result in greater computation time. This generally translates into an increased level of effort and expense in model construction and validation and computing costs.

7.3-3.2 Finite Element Technique

If the geometry or internal physical features are curvilinear, then it might be easier to model the aquifer using a finite element approach with triangular elements of varying size as depicted in Figure 7-1(d). Irregular aquifer or lateral internal variations in geologic properties (e.g., lateral changes in aquifer properties or irregularly shaped water bodies) can be more readily accommodated with a finite element mesh although the time necessary to construct the grid and input the data into the computer can be considerable.

The finite-element method approximates differential equations by an integral method. The model area is divided into sub-regions, or elements, and the finite-element model grid may consist of triangles or quadrilaterals. Numerical models utilize a variety of solution techniques to solve the resulting equations. Additional information on finite-difference and finite-element techniques and solution techniques is contained in numerous introductory modeling texts (e.g., Wang and Anderson, 1982; Walton, 1985).

7.3-4 Solute-Transport Models

Solute-transport models simulate the distribution of contamination as concentrations (i.e., mass per unit volume of a compound) in an aquifer by simultaneously solving both the flow equation and the transport equation. Physical, chemical, and biological processes all affect the rate and migration of contaminants in an aquifer.

Solute transport processes include physical phenomena, and chemical and biological reactions. Individual processes are, in some cases, fairly well understood under laboratory conditions and can be somewhat replicated under field conditions in saturated porous media. Solute transport in fractured bedrock is much more difficult to identify and characterize because of the heterogeneous anisotropic nature of the aquifer. In addition, when multiple contaminants are present that respond differently to different processes in either media (unconsolidated or bedrock), the resulting synergistic reactions become difficult to model. Thus, real problems arise in very heterogenous or fracture-dominated systems or when nonaqueous phase contaminants or solutes that react with solid, liquid or biological components of the subsurface are present. These cases, and they are common (i.e., gasoline spills, metals, organic solvents, etc.), can be very difficult to model. Consequently, this greatly limits the reliability of using mathematical models of solute transport to predict future site conditions for such situations.

The basis for the selection of values of various input parameters for solute transport models, such as dispersion coefficients, is still being debated. Another required input parameter, which is generally not well defined, is the strength of the contaminant source. Also, input parameters for the transport equation, such as dispersion coefficients and biotransformation rates, are difficult to quantify in the field with available technology, particularly in groundwater regimes where flow is very slow.

Assessment of solute transport requires a multi-disciplinary approach that integrates the geologic, hydrologic, chemical, and biologic processes and features that are important at a site (Keely, 1987). A complex array of chemical wastes and a poorly documented contaminant release history are associated with most contaminated sites, thus making solute-transport modeling a difficult proposition. Some of the known factors that influence the fate and transport of contaminants are listed on Table 7-1. At the present time, there are many gaps in our understanding of solute-transport phenomena and the appropriate methods for characterizing them.

Of the physical processes affecting solute transport, advection, a flow dominated process, is the most well understood parameter. Recent studies (Sudicky, 1986) indicate that advection may be the dominant control in the physical processes of solute transport and that the delineation of the complex and difficult-to-measure parameters such as dispersion or diffusion may be unnecessary. These studies suggest that a detailed description of the distribution of hydraulic conductivity in an aquifer may be the most important factor in simulating solute-transport, although obtaining this data could be economically prohibitive. Hence, in order to predict contaminant transport adequately, it is imperative to have a well-calibrated groundwater flow model. Other researchers, however, suggest that calculations of travel time based solely on advection and longitudinal mechanical dispersion may greatly underestimate breakthrough of the solute (Keely, 1987). Finally, under certain circumstances, for example, when flow velocities are extremely low (e.g., when leachate passes through clay liners), molecular diffusion becomes the controlling component for solute transport, unless there are conduits for vertical flow through the clay liners such as cracks, roots, etc..

The measurement and mathematical description of chemical processes in the subsurface are less certain than the physical processes affecting solute transport. Although parameters such as ion exchange and oxidation-reduction reactions are well understood in the laboratory, their application to field conditions is difficult. In addition, the complex interaction of various organic and inorganic compounds that are often present at contaminated sites is difficult. The solute-transport models currently available do not take these chemical and geochemical interactions into account.

Biological processes are another set of frequently overlooked parameters that affect the fate and transport of contaminants. These processes include the biotransformation of one compound into another as the result of subsurface biological activities. Although the presence of these processes is recognized, the factors influencing the rates, abundance, and impact of these processes are not well defined. The effect of biological processes on solute fate and transport is currently an area of intensive research and, as these processes are better quantified in the field, they may be able to be more accurately modeled.

Due to the complex nature of the interactions of these processes, it is often necessary to make assumptions and simplifications to obtain mathematically manageable solutions (Keely, 1987). In many cases, the impact of certain parameters must be ignored completely in order to describe the problem mathematically. The magnitude of errors arising from these assumptions and simplifications must be carefully evaluated.

For example, transport models, which only consider advection and dispersion, are not likely to be representative of a case where contaminants may be removed by a process such as adsorption. Consequently, the accuracy and applicability of solute-transport model simulations must be reviewed in light of the assumptions made during the modeling phase. Until there is a better understanding of all the subsurface processes affecting solute transport, the results simulated by solute-transport models should be applied with caution when making remedial and/or regulatory decisions with regards to a site. Use of conservative values for transport parameters can, however, establish reasonable limits to expected concentrations. Under worst-case conditions, it may be possible to establish acceptable risk criteria for a site.

7.3-5 Application of Numerical Models to Groundwater Flow Problems

Numerical models can be applied to a variety of groundwater problems to increase the user's understanding of the natural flow system and how the flow system might respond to various stresses, both natural and man-made. Models can be used either for interpretive or predictive purposes to simulate how a particular aquifer may respond to recharge, pumping wells, or some other form of hydraulic remedial action. Models can also be useful tools for designing a subsurface monitoring program for site investigations or long-term monitoring. Typical applications of numerical models include:

- Testing and improving the conceptual model of a ground water flow system initially formulated on the basis of field observations;
- Evaluation of the impact of various activities on groundwater quantity (aquifer stress and yield);
- Evaluation of the effectiveness of alternative remedial pumping schemes;
- Evaluation for risk assessment purposes of the potential exposure of receptors to various contaminants over time;
- Definition of well head protection zones;
- Evaluation of saltwater intrusion; and
- Design of monitoring well networks.

7.3-6 Modeling Limitations

An important step in any modeling program is to determine if the construction of a mathematical model is appropriate and necessary. Figure 7-2 is a flow chart for determining whether or not modeling is required. Often times, gathering additional data will improve the conceptual understanding of the site; however, a cost benefit analysis that considers the goals of the investigation should be performed prior to collecting more data.

In some cases, models are used to predict current groundwater contaminant concentrations at potential exposure points, utilizing only data near the contaminant source. Project managers should constantly evaluate whether simply gathering real, current data at the potential exposure points is useful and beneficial.

Because of the sometimes extreme heterogeneity of the geologic environment or the potential for different interpretations of the same hydrogeological data set, a good modeler should always take a conservative approach in evaluating the validity of the model in its ability to estimate some prior or future condition. Embarrassing stories abound in modeling circles concerning the discovery of previously unidentified geologic features identified with subsequent drilling programs, which, by their presence, necessitated major revisions to the conceptual and numerical model. Models aid in understanding how a system works, but room for refinement of that understanding always exists.

7.4 PROCEDURES FOR CONSTRUCTING A NUMERICAL FLOW MODEL

7.4-1 Modeling Team

At a minimum, the modeling team should consist of the modeler and the site geologist/hydrogeologist or engineer skilled in groundwater hydrology. The site project manager need not be a geologist/hydrogeologist. The modeler should conduct one or more site visits and frequently discuss the model with the site geologist/hydrogeologist with regards to where he/she feels the weaknesses of the model exist and what kind of information he/she needs to strengthen the model. Under no circumstance should the modeler construct the model without consulting with the site geologist/hydrogeologist, unless he/she is also the site geologist/hydrogeologist or has conducted the field work.

The model selected for use on a project should vary according to site conditions and modeling requirements. The level of experience of the modeler should also vary with the more experienced modelers constructing the more complex models. Depending upon the size and complexity of the model and staff availability, a less experienced modeler should serve as an aid to the principal modeler assisting in grid construction, data entry and performing the computer runs. In this way he/she gains more experience in learning how to construct and calibrate more complex models.

If a solute transport model is also required, then depending upon the contamination that is being modeled, a chemist in the particular branch of chemistry in question should be part of the modeling team. That individual should review the geologic and chemical data and participate in the development of the conceptual model. The types of contaminants that can be modeled include:

- inorganics (including metals);
- volatile organic compounds;
- acid/base neutral compounds;
- dense or light non-aqueous phase liquids (DNAPL or LNAPL, respectively); and
- radioactive compounds.

All of these classes of compounds have different physical, chemical and biological properties and will behave and react differently in the aquifer and in some cases with each other as well. For some chemicals (e.g., for a DNAPL plume) and/or some aquifer conditions (i.e., fractured bedrock) acquiring sufficient data could be extremely difficult.

Another important requirement for a modeling program is time. Where analytical models may take an hour or a day to set up and evaluate, numerical models, depending upon their size and complexity, may require weeks or months to properly design and calibrate.

7.4-2 Conceptual Model

The conceptual model is the modeler's and project geologist/hydrogeologist's concept of how the physical hydrogeological system works. It includes a discussion of all of the controlling factors in the system, such as aquifer extent and thickness, sources, sinks, and hydrogeologic boundaries. Alternatively, it may be a working hypothesis that the modeler wishes to test. In addition, the conceptual model becomes the basis for developing future data gathering efforts. Any model is only as good as the conceptual model and its ability to capture the essential elements of the hydrogeologic system.

A conceptual model should be developed whenever a site is being evaluated irrespective of whether or not a model is to be constructed. It is a "picture" in the project manager's mind of what the site subsurface and groundwater flow conditions are. It is, or should be, continually refined as new data are acquired. The development of a conceptual model should begin as the first pieces of information are received. Activities as rudimentary as review of a topographic map, hydrologic atlas or conducting a site visit should begin to stimulate ideas or "concepts" about the site hydrogeology. As more data is gathered and reviewed (e.g., aerial photographs, boring logs, prior reports, etc.), the site geologist/hydrogeologist should continually be refining his/her mental image of the aquifer. The evolution of the conceptual model is the primary responsibility of the site geologist/hydrogeologist not the modeler. The site geologist/hydrogeologist synthesizes all of the data and presents the conceptual model to the modeler for review and discussion. The modeler then reviews the conceptual model and depending upon the goals the modeling effort may have some specific data needs or requirements in order to fulfill those goals. The subsequent field work initiated for the project should, costs permitting, attempt to fulfill those goals.

Very often contamination exists at the site (i.e., a leaking UST, a lagoon, a waste pile). A conceptual model of the waste source and its migration pathway(s) to the subsurface also needs to be developed simultaneously and integrated with the conceptual flow model. This should be done irrespective of whether or not a solute transport model is to be constructed as it will aid in locating monitoring wells or sampling locations.

Whatever the type of model to be constructed or used (i.e., analytical or numerical), a conceptual model of the aquifer needs to be created. As dictated by the site complexity and level of effort requested by the private party or DEP and the goal of the modeling effort, the conceptual models should include, but not be limited to:

- sketches;
- cross-sections;
- block diagrams;
- flow nets in map view and in cross-section;
- aquifer geometry;
- distribution of geologic materials both laterally and vertically;
- nature of the underlying bedrock;
- description of lateral aquifer boundaries (i.e., valley walls, streams, etc.);
- a discussion of major withdrawals or recharge to the aquifer;
- leakage from overlying bodies of water;
- wetlands or underlying aquifers;
- the nature of any confining units that might be present;
- the gaining or losing nature of any streams or rivers within or adjacent to the aquifer;
- horizontal and vertical hydraulic gradients;
- hydraulic conductivity and storativity of the different geologic materials in the aquifer; and
- the distribution of natural recharge across the aquifer.

In general, the more complex the site, the greater the level of effort is required to evaluate its hydrogeology and the more detailed is the conceptual model with fewer simplifying assumptions. Conversely, a simple site requires a lower level of effort and results in a less detailed conceptual model. Modelers should not extend a limited data set in order to achieve results for a complex set of goals.

7.4-3 Selection of an Appropriate Model

The selection of the type of model should be based on the objectives of the program, the complexity of the system, and the available data. According to de Marsily (1986), situations where the construction of a numerical model may be more suitable than an analytical model include:

- needing to identify migration pathways and predict end point receptor concentrations;
- having boundary conditions (either flow or no-flow) with complex shapes and/or situations where assuming infinite areal extent, constant aquifer thickness, and homogeneous, isotropic conditions or the use of image wells cannot adequately describe the system;
- having a non-linear problem where no analytical solution is available.
- varying aquifer geometry that is too intricate to be adequately represented with an analytical model, i.e. single values of hydrogeological parameters selected for the analytical model are inadequate for describing the real system; and/or
- having an analytical solution available, but which is very time-consuming or complex to calculate.

Selection of the most appropriate numerical model should be based on site conditions, the purpose of the modeling exercise, and the availability of data to adequately construct and calibrate the model. For example, a two-dimensional (2-D) groundwater flow model is appropriate if groundwater flow can reasonably be assumed to be horizontal. In constructing a 2-D model, if vertical heterogeneities exist in the aquifer, vertically averaged values of hydraulic conductivity can be calculated and used as input data. A cross-sectional or profile model can be constructed when consideration of vertical flow is important. The profile, however, needs to be constructed along a flow line.

A three-dimensional (3-D) model is appropriate if flow or solute transport in the third dimension is important to the understanding of the site hydrogeology (e.g., during pumping simulations in the vicinity of the pumping well, or where leaky aquitards are present, where the vertical distribution of head is of major interest, or where significant vertical heterogeneities exist). Three-dimensional models are also very useful in areas where groundwater flow is controlled by topography which may give rise to the presence of local, intermediate and regional flow systems resulting in complex vertical flow conditions.

For any numerical modeling effort, however, there must be sufficient data collected to support its construction, calibration and validation. Obviously, when constructing a three-dimensional model, the data requirements are significantly greater than for a two-dimensional model. For example, a number of well nests or well clusters are necessary in order to calibrate a 3-D model which greatly increases the cost of the field effort and the length of time necessary to complete it.

When aquifers that have vertical variations in composition and/or have vertical differences in hydraulic head or situations where it is important to know the vertical distribution of head are going to be modeled three dimensionally, multi-level or multi-port wells need to be installed in areas where vertical changes in head are anticipated. Not only is this an expensive and time consuming process, but constructing, calibrating and verifying a three dimensional model becomes very time consuming and expensive as well. For these situations, there has to be an extensive amount of field work of sufficient adequacy to achieve the desired objective.

What constitutes a "sufficient" data set is a matter of interest that deserves some discussion. Geostatistical software packages are available that are used for parameter estimation. "Kriging" is just one of a handful of techniques that is used to take a known data set and interpolate between those values as well as assign a confidence interval for the estimates that have been calculated. Another way of kriging data is to evaluate the data set of a number of values from one well (e.g., water quality) to arrive at a value that is representative of the entire set. Another way of stating the above is that kriging is the process of finding the best linear unbiased estimate at a point (or the average over an area) by linear interpolation from the variable data (DeMarsily, 1986).

The confidence interval of the estimate will vary depending partly upon the number of samples. The data sets for hydrogeologic investigations for the most part are rather limited. Consequently, the estimated confidence interval needs to be looked at carefully. For example, interpolation of a water table data set for an unconfined aquifer (i.e., a water table map) and a map showing the areal distribution of hydraulic conductivity might have similar confidence intervals. However, given the nature of the two parameters, hydraulic head (which spatially varies fairly uniformly and is rather damped) and hydraulic conductivity (which may be randomly distributed), the contoured map of piezometric data is less likely to significantly change with the acquisition of new data than the hydraulic conductivity map.

7.4-4 Data Compilation

A significant amount of data is needed to construct an accurate numerical model. Typically, a model begins with the construction of a series of maps and stratigraphic cross-sections that describe the aquifer conditions. This information is generally compiled by members of the field investigation team or modeling team and has as its basis the conceptual model that has been developed for the site. Because the conceptual model evolves continually, it is not unusual for the conceptual model to be refined as the data is compiled and depicted in the various types of maps and figures that hydrogeologically describe the site. Input data for a numerical model usually consist of, at a minimum, the items described below.

7.4-4.1 Geometry of the Aquifer System

The geometry of the aquifer system consists of a physical description of the aquifer including the geologic units, their vertical thicknesses and lateral extent. This information is obtained from subsurface borings, surface and borehole geophysical data, surficial mapping, an understanding of the geomorphology and depositional environment, and the construction of geologic cross-sections.

A minimum number of contoured maps should be developed prior to model construction. For a water table aquifer, they are:

- a hydraulic conductivity map;
- an aquifer bottom elevation map (this may or may not be equivalent to a bedrock topographic map;
- a land surface topographic map;
- a map of the elevation of water table; and
- a porosity map, if solute transport is being modeled.

For a confined aquifer, maps depicting the lateral distribution of transmissivity (rather than hydraulic conductivity) in the aquifer and the potentiometric surface are required. In some cases (e.g., transient flow modeling), maps depicting the distribution of specific yield (water table aquifer) or storativity (confined aquifer) may be required. This latter information is generally difficult or expensive to obtain in the field and globally assumed values from published literature are often used in the model. However, depending upon the types of geologic materials present, it may be desirable to use different published values in different parts of the aquifer (e.g., till upland adjacent to stratified drift).

It is not unusual for modelers to use equations for confined aquifers to estimate responses in unconfined aquifers (i.e., holding transmissivity constant), particularly if the dewatering effects in the area of concern are minimal. (Note: dewatering lowers the water table and reduces the saturated thickness, which in turn results in a lower transmissivity.) The advantage to doing this is that data compilation and entry time are significantly reduced. This approach is more acceptable in regions that are distant from a pumping or recharge well or where seasonal changes in the water table are small. The model will accurately reflect head values in those areas. Where dewatering is significant (greater than approximately 10% of the saturated thickness), this approach is not recommended and should not be used without correcting the drawdown for the dewatering effect.

7.4-4.2 Transmissivity

The transmissivity of the aquifer can be obtained directly from pumping tests as well as from other methods. In order of preference, they are:

- pumping tests,
- field tests of hydraulic conductivity (i.e., slug tests),
- dividing estimated regional flow by measured hydraulic gradient,
- laboratory permeability tests on the soils,
- grain size analysis, or
- published data.

When hydraulic conductivity (K) is obtained directly (i.e., slug tests, grain size, etc.), the saturated thickness of the aquifer (b) must be estimated so that the transmissivity (T) can be calculated (T=Kb).

Pumping tests, particularly large capacity tests, are the preferred way to estimate transmissivity over large regions of the aquifer. Transmissivities derived from pumping tests are less satisfactory for solute transport models where variations in hydraulic conductivity are more important than average conductivities over a large region. Very often in dealing with contaminated sites, pumping tests, prior to the treatment system being operational, are run at much lower volumetric rates to minimize the extraction of contaminated groundwater and consequently impact a smaller region of the aquifer. Slug tests measure the hydraulic conductivity only in the immediate vicinity of the monitoring well and care must be taken in extrapolating those results very far from where the measurements were taken. Regional flow can sometimes be approximated based on estimates of areal recharge and the upgradient recharge area. Using Darcy's Law, this flow can be divided by the measured gradient and flow tube width to approximate transmissivity. Laboratory tests for hydraulic conductivity require physically taking samples of the aquifer into a soils lab for permeameter testing and/or for sieve analysis (see Section 3.8-1). In doing this, the soil structure (packing) is disturbed which will alter the hydraulic conductivity. In the absence of field data, published tables may provide reasonable estimates of hydraulic conductivity.

7.4-4.3 Storage Coefficients

The storage coefficients and/or specific yields are also necessary input parameters for transient simulations. Storage coefficients can be determined through aquifer tests, and specific yield can be estimated through aquifer or matrix and void space volumetric tests that are performed in the laboratory. If these data are not available, assumed values for these parameters are often used. An order-of-magnitude value is often assumed for the confined storage coefficient. Specific yield or unconfined storage coefficients can be estimated much more closely.

7.4-4.4 Identification of Surface Water Features

The locations of surface water bodies are also necessary for model construction. Locations usually can be obtained from topographic maps or from aerial photos, although more accurate information regarding these features is generally obtained in the field. The hydraulic connection and flux (i.e., leakage, induced infiltration, or groundwater discharge) between these surface water features and the groundwater system will need to be quantified.

7.4-4.5 Leakage

Leakage rates from semi-confining layers, or induced infiltration or leakage from lakes, ponds and streams can be determined by analyzing data from a well-designed aquifer test or estimated from the geologic description of the adjacent units, based on their estimated thickness, permeabilities, and vertical head differences. Seepage meters and streambed piezometers can also be used to quantify flux from an adjacent surface water body into or out of an aquifer (Lee et al., 1978).

7.4-4.6 Delineation of Discharge and Recharge Areas

Depending upon the goal of the modeling effort, the location and rate of recharge to the system through precipitation, infiltration, and or injection should be determined based on field measurements or estimated from available geologic and climatological data. Zones where groundwater is extracted from the aquifer system through pumping or natural discharge to surface waters should be identified and quantified to the extent possible. Measurement of pumping rates and temporal variations in pumping rates from wells and the use of stream-gauging and seepage meters in streams and swamps can provide data to help quantify these factors.

7.4-4.7 Piezometric Heads

Piezometric head data are required for the construction, calibration, and validation of a model. These data are obtained from water-level measurements made at various locations and depths in the aquifer. This information can be compiled in the form of water-table and piezometric maps or hydrographs for specific wells. The collection of head data over a period of several years may be required to determine long-term (steady-state) conditions in an aquifer. For 3D models, piezometric measurements should be made in all aquifer layers that are being modeled in order to achieve a good calibration.

It is not unusual for a site to be investigated over a period of years with the modeling effort coming in the later part of the project. Consequently, it behooves the project manager to have water levels measured at a minimum on a quarterly basis until the hydrogeology is understood. Once that occurs, semi-annual measurements (preferably in late spring and fall) can be taken. The U.S. Geological Survey (USGS) has a network of long term monitoring wells in the state that are measured on a monthly basis. This data should be used, when appropriate, to supplement site-specific data. Techniques for predicting probable high groundwater levels in Massachusetts and on Cape Cod are available from the USGS (Frimpter, 1980 WRI-OFR 80-1205 and Frimpter, 1980 WRI-OFR 80-1008, respectively).

7.4-5 Definition of Boundary and Initial Conditions

In order to solve the partial differential equations that define the flow regime, the nature and location of the hydrologic boundaries need to be determined. This information may be based initially on a conceptual model of the flow system, however, the existence of boundaries must be verified in the field. Models should maximize the use of any field measurements of stream and pond elevations, or discharge and recharge rates, as well as the physical location of aquifer boundaries. When transient conditions are simulated, initial conditions are also required. For example, in a simulation of flow through an unconfined aquifer, the initial piezometric head values are assumed at the node locations within the aquifer. These head values represent the initial conditions for the transient (non-steady state) simulations.

In some cases the natural limits of the aquifer may be extremely far from the area of interest in the model. In this case artificial boundary conditions may be used, such as constant-head (i.e., an equipotential line), constant flux, or no-flow boundaries (i.e., a groundwater flow line). In applying these artificial boundary conditions to the model, it is assumed that these boundaries will not be significantly affected by the simulation. If pumping or recharging wells are influencing these boundaries, then the model will need to be reconstructed so as to minimize this interference. The appropriateness of these boundary conditions should be checked to determine their influence on long-term predictions of the model (de Marsily, 1984). This can be accomplished by replacing a constant-head boundary with a specified-flux boundary and running the model again. If the differences in the two simulations are insignificant, then the artificial boundary conditions are not significantly affecting the simulation. Note, however, that the model still might not be valid due to failure of other criteria, which are discussed in Section 7.6-3, Sensitivity Analysis.

7.4-6 Construction of the Model Grid

Once the conceptual model has been formulated, the model grid can be constructed. This process is often referred to as discretization. The design of the grid will affect the accuracy of the piezometric approximations at specific locations in the model, as well as the amount of time necessary to run the model on a computer.

A general rule of thumb to follow is that if variable grid spacing is to be used, then the node or grid spacing should become smaller whenever there are abrupt changes in: 1) physical properties (e.g., a till-stratified drift contact); or 2) piezometric head (e.g., adjacent to a production or recharge well). Referring to Figure 7-1(a), (c) and (d), the node spacing in the vicinity of the production wells is much closer than along the model boundaries. The closer grid spacing will provide better resolution of piezometric head in those areas. The trade off for having a finer grid spacing is that in doing so, the number of nodes generally increases which results in greater computational time. This may seem insignificant for a two dimensional model, but can become significant for three-dimensional models. This can be compensated to some degree by creating larger grid spacing away from the areas of interest (e.g., near the model boundaries (see Figure 7-1(d)). With regards to node spacing, some finite difference codes recommend that an adjacent node be no more than 1.5 times the distance between the last two nodes.

The following general guidelines (modified after Mercer and Faust, 1981) should be followed when designing a model grid:

1. Place nodes at pumping centers and monitoring/observation wells. In the case of a tubular well field (i.e., a series of small diameter wells manifolded together), a number of wells can be grouped together at one node.

2. Accurately locate model boundaries so that they correspond with real hydrogeologic boundaries. As depicted in Figure 7-1, finite element techniques can approximate curvilinear boundaries and other features better than finite difference techniques. The loss of this kind of detail is not significant if knowing exact piezometric heads in those areas is not important.

3. Place nodes close together in areas where there are large variations in geologic conditions or anticipated, significant changes in hydraulic head (for example, near pumping or recharging wells). What defines "close" is really a function of the size of area to be modeled, the number of nodes that are available, and the particular solution technique utilized in the code. The larger the area, the greater the node spacing. The limiting factors are either the software (some codes have a 2,500 node limit) or the hardware (available memory capability).

4. Align the axes of the grid along major directions of anisotropy or heterogeneity.

7.4-7 Assignment of Parameters to Nodes

Once the basic data have been compiled and the model grid has been designed, model parameters can be assigned to each node. At this point, the physical aspects of the aquifer are defined for each node in the model by overlaying the model grid over maps of saturated thicknesses, transmissivity, initial conditions, and other features. The properties are assigned to each node of the model and comprise the input files for the model.

Keying the data into the computer on a node-by-node basis is a time consuming process and incorrect data can often be entered for a node. It is important to check the input data very carefully prior to running the model. It is pointless to attempt to calibrate the model if the input data is in error. Some errors become apparent only when first attempting to run the model, particularly when using a new or unfamiliar model. The user should plan on some initial debugging runs to aid in correcting input data files.

7.5 PROCEDURES FOR RUNNING A NUMERICAL FLOW MODEL

7.5-1 Model Calibration

Calibration of the model consists of running the model and comparing model-simulated heads to a set of field-measured heads and, where applicable, model-simulated rates of groundwater discharge to a set of field-measured rates of groundwater discharge. This is accomplished through a trial-and-error process of varying aquifer parameters (e.g., transmissivity, storativity, recharge, etc.) in different regions of the model (having, of course, some justification for making the changes) until the match between model-simulated and field-measured conditions is considered acceptable. Calibration can be performed to steady state or average head conditions or to transient conditions. Other calibration criteria include a water mass balance, groundwater discharge to streams (i.e., gain or loss), and, if the model is a three dimensional one, vertical and horizontal head distributions in all layers.

There is no textbook definition of what constitutes an "acceptable" match between simulated and measured data. Simulated data will rarely exactly match measured data, however, the difference between the two should be minimized. Two methods of comparing simulated to measured data are to calculate the absolute average difference (AAD) or to calculate a standard deviation and root mean square error (RMSE) for all the data. If the standard deviation and the RMSE is small or if the AAD is small, then the calibration is considered acceptable with the following exception.

There will invariably be outliers, that is, locations or nodes where the difference between simulated and field data is substantial. If those nodes are in central areas of the model where predicting heads for future scenarios is desired, then the model calibration should not be considered "acceptable". If, however, those nodes are distant from where forecasting information is sought (e.g., a till upland region adjacent to the aquifer), then this difference often times will have little impact on the modeling results.

A word of caution against too finely tuning a model may be justified here. A more generalized model that calibrates reasonably well may be more valid than one in which the RMSE is very small, but its parameters have been very finely tuned in areas where there is no field data to verify that these changes are warranted.

Also, care must be taken when constructing the model using interior constant head nodes. A river or lake that is large enough and in good hydraulic communication with the aquifer may be represented with a series of constant head nodes. However, if a water body is shallow and susceptible to large fluctuations in water level elevation, constant head nodes may not be the best representation.

A detailed log of the adjustments that have been made to the input data during the calibration process should be maintained. This will provide a record of the modifications made to the original entries and should help to avoid repeating calibration runs. During the calibration phase, the modifications should be checked against the original conceptual model to ensure that the model is still representative of the physical system. It is easy to stray from the original concept of the system during the calibration process.

The reliability of the model is related to the accuracy with which the model simulates field conditions. It is important to keep in mind, however, that just because the model reproduces one set of field conditions does not mean that it is valid. Modification of different sets of parameters can produce similar solutions. Consequently, the calibration of the model must be performed systematically and with a good understanding of the site conditions. For a particular site, given the proper assumptions, additional field data will often improve the accuracy of the model. Many times it is necessary to perform additional field work to fill in data gaps before an accurate model is obtained. The decision to obtain further data must include a careful weighing of benefit to the model (reflecting model goals) and cost and time involved in obtaining the additional data.

7.5-2 Model Validation

Upon conclusion of the calibration process, the model should be run with a different set of initial conditions produced by a different set of stresses than the initial calibration (e.g. high vs. low water table or pumping vs. non-pumping conditions). Because of the non-uniqueness of the solution, the model should be validated with as many sets of initial conditions as may exist prior to using the model for any forecasting. Preferably, data should be collected at periods of seasonally high and low water tables in order to reflect seasonal fluctuations in recharge and surface and groundwater conditions. Confidence in the reliability of the modeling predictions can only increase as a result of this exercise although no model can ever be fully validated. See Van der Heijde (1986) for a more detailed description of validation procedures.

7.5-3 Sensitivity Analysis

Once a model has been calibrated and validated, a sensitivity analysis should be performed on the model. This is accomplished by varying the values of input parameters where there is little field control and evaluating the resultant distribution in heads. If the model is very sensitive to reasonable changes in a parameter value (e.g., transmissivity, recharge, leakage), then caution should be exercised in interpreting results from the model, particularly under applied stresses differing from calibration conditions. Depending upon the importance of the forecasting capability of the model, (i.e., does the possible range of outcomes preclude adequate selection of alternatives or prediction of impacts), more field work may be required to decrease the uncertainty of the model in that area.

If the area where the uncertainty exists is in a remote part of the modeled area, determining more precise physical conditions may not be necessary. Leakage from or to a stream, however, may greatly alter head levels in an adjacent production well and hydrogeologic data will need to be more accurately quantified in that area. A sound conceptual model will aid in identifying sensitive areas early on in the program.

7.5-4 Forecasting

Upon completion of the calibration and verification procedures and at the conclusion of performing the sensitivity analysis, the model can be used to simulate past, current, and/or future conditions. One advantage of a numerical model is that, once calibrated, it can be used to simulate a variety of situations. A flow model can be used to predict the response of an aquifer to conditions of average or excessive recharge or to a drought. If a model is being used for long-term planning and prediction, it should be periodically recalibrated as new data becomes available. Caution should be exercised in attempting to use the model under conditions much different than those under which it was formulated and calibrated/validated.

7.6 REPORTING MODEL RESULTS

7.6-1 Presentation of Results

An important but often overlooked aspect in the use of groundwater models is the proper presentation of modeling results. In order to present modeling results in a systematic, clear and effective fashion, the following format is suggested. This format is an adaptation of the DEP Division of Water Supply's published Policy 87-12, "Quality Assurance for Groundwater Modeling".

7.6-2 Purpose

State the purpose, goals, and objectives of the modeling effort.

7.6-3 Conceptual Model

Develop and present a conceptual model of the aquifer system and, if applicable, the contamination problem of concern (i.e, existing distribution of contaminants and source characteristics). This should include cross-sections and maps of the geology and hydrology of the aquifer at an appropriate scale, including maps of the areal extent of the aquifer and if applicable, distribution of contamination, saturated thickness, water table and boundary conditions maps. Present pertinent available data with a discussion of their deficiencies.

7.6-4 Data Collection

Explain how, when, and by whom the data were collected, analyzed, and interpreted. Exploration methods and data-analysis techniques should be presented. The level of confidence in resulting parameter identification should be described. Describe how model results may be limited or restricted by the lack of knowledge about key aspects of the hydrogeologic system.

7.6-5 Model Description

Document the groundwater flow and contaminant transport model (software) that is being utilized. Include such information as the model name, its author(s) and the purpose for which the software was developed. The use of well documented and tested software is recommended over the use of custom or altered software. If an altered code is utilized, it should be thoroughly tested against a variety of known analytical solutions. The documentation must include the governing equation(s) being solved.

Explain why the model being utilized was chosen. All simplifying assumptions inherent to the application of the model should be stated and justified, as well as the impact these assumptions may have on model results. A comparison between these assumptions and actual conditions should be made. Describe where model assumptions and actual field conditions do not coincide and how this may affect model results.

7.6-6 Assignment of Model Parameters

All initial conditions, boundary conditions, hydraulic and transport parameter values should be defined and the reasons for selecting these conditions justified. The values assigned throughout the modeled area should be presented. The area covered by the model should be presented as an overlay on a topographic base map of appropriate scale, highlighting boundary conditions and hydraulic parameter values.

7.6-7 Model Calibration

Model calibration goals and procedures should be presented and discussed. The results of the final calibration run should be presented and analyzed and departure from the calibration targets analyzed. The effects of these departures on the model results should also be discussed.

7.6-8 Model Validation

If model validation has been performed, its goals and procedures should be presented and discussed. The results of the validation run should be presented and analyzed. Important points include departure from the validation targets and the significance of these departures. Present and discuss the overall model water and chemical balance, highlighting salient features of the model scenario (e.g., pumpage, recharge, leakage, or boundary conditions). Ideally, the validation should consist of a single run (per validation data set). If the validation run is not successful, but information is obtained of a suitable nature, it may lead to re-evaluation of the conceptual model and possible changes and further calibration.

7.6-9 Sensitivity Analysis

Model sensitivity analysis should be presented and interpreted. Determine what parameters of the model have the greatest influence on the model results. The analysis should focus on those parameters that utilize the least certain assumptions. Also indicate, on the basis of the sensitivity analysis, what the emphasis of future data collection efforts should be best to improve the model.

7.6-10 Data Preprocessing and Postprocessing

All preprocessing of model input data must be thoroughly described. Special precautions to avoid data input error must be applied and described. All postprocessing of model output data must be thoroughly described and any computer codes utilized must be documented. Note vertical exaggeration in any computer-generated cross-sections.

7.6-11 Model Prediction

The model output from all predictive scenarios should be presented and interpreted. Present and discuss the overall model water balance for each specific forecasting scenario. Show results in terms of new head distributions, rates of groundwater discharge, distribution of concentrations, and so forth. Discuss how model sensitivity and uncertainty could affect the predicted results.

7.6.12 Model Results

The physical reality of the model should be discussed (i.e., how well does the model represent the physical and chemical processes of the environment being simulated?). Restate the fundamental assumptions in the presentation of the model predictions. Note if the model results support the initial assumptions described in Section 7-7.4.

The model results should be presented both in technical and non-technical (i.e., layman's) terms. Model results should also be qualified, for example: "Given conservative values, within the range of expected variation, the model results show..." or "Given less conservative values within the range of expected variation, the model results show...".

7.6-13 Model Records

The modeler should provide/keep the following records on file in digital form:

- The version of the source code utilized;
- Input parameters, boundary and initial conditions;
- The final calibration run (input and output files); and
- All predictive runs (input and output files).

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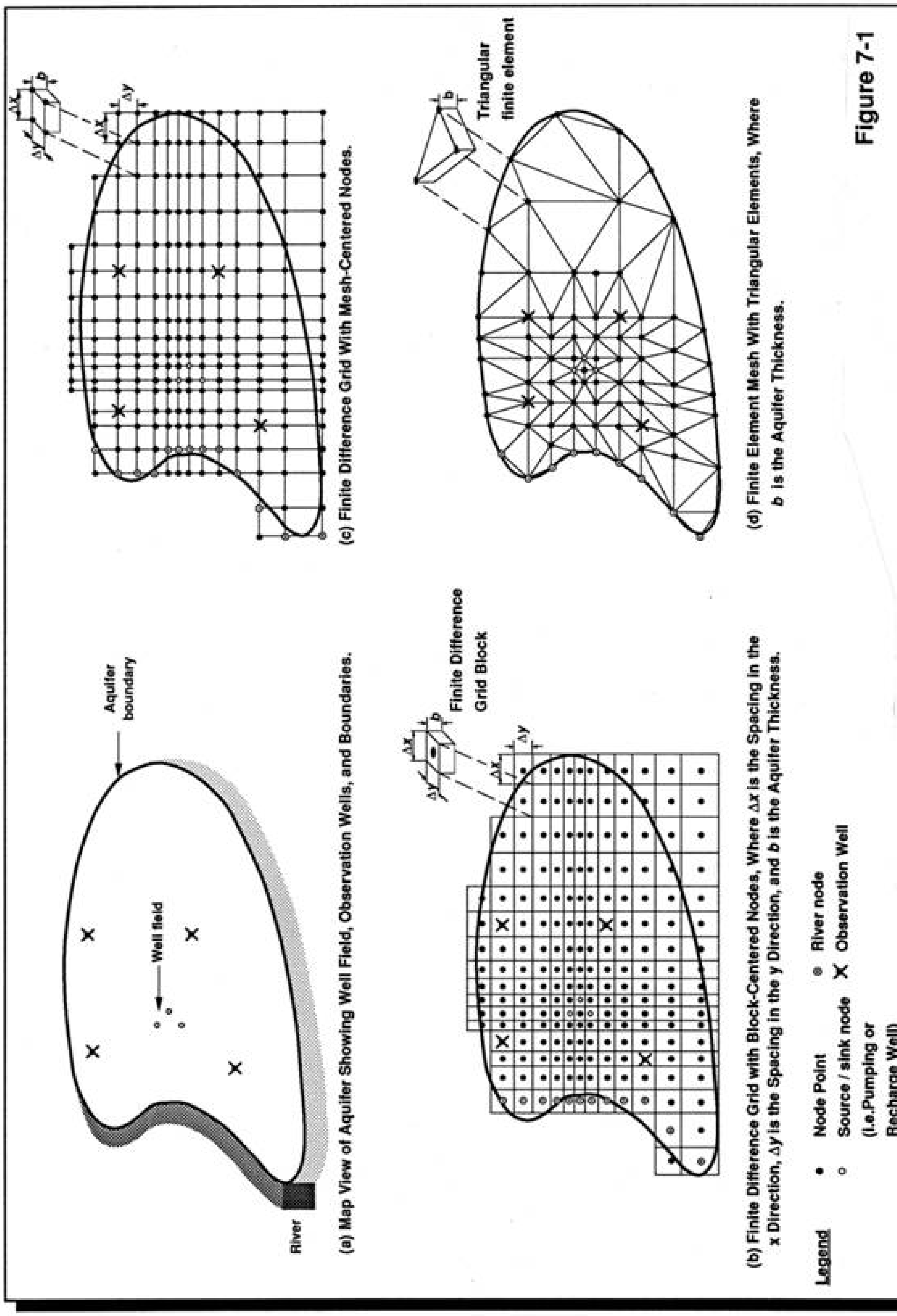
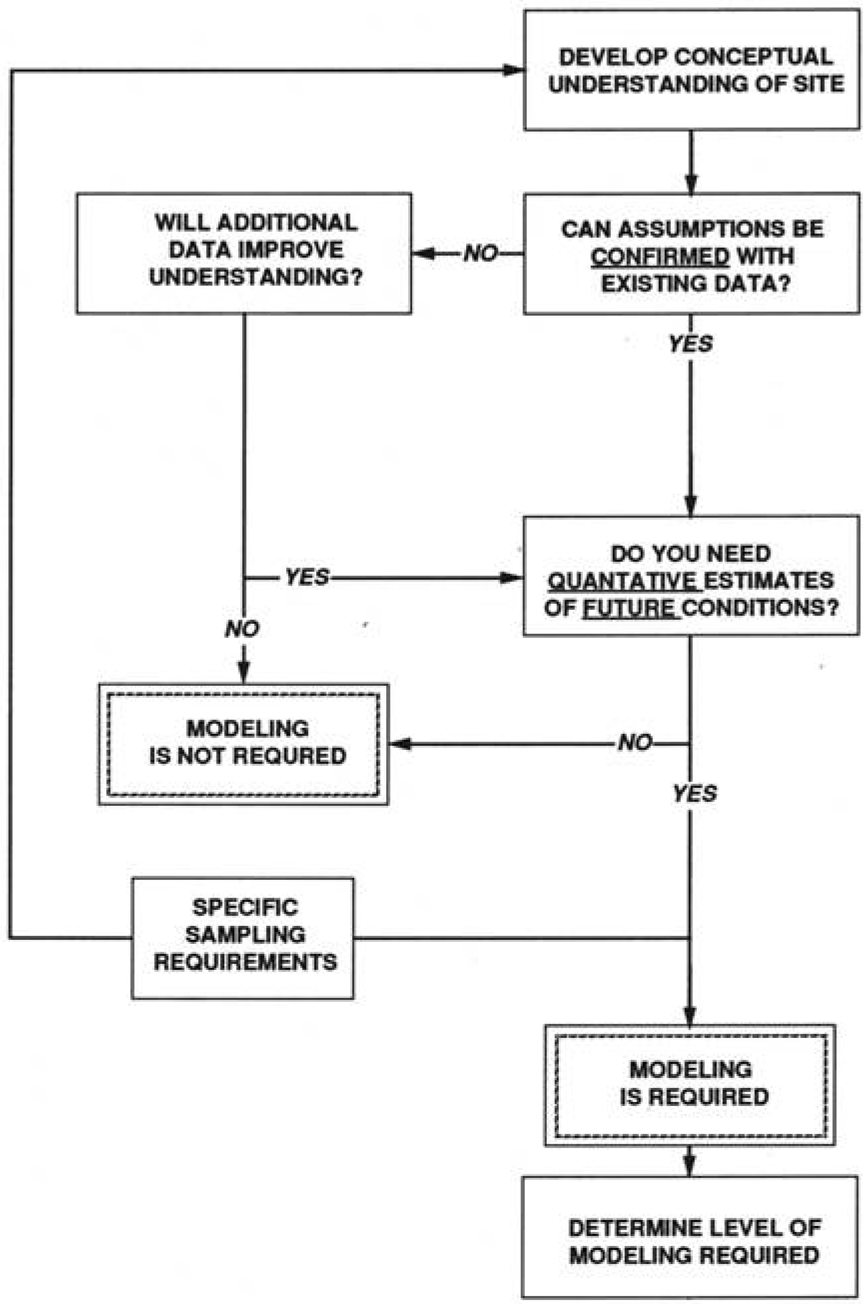


Source: Adapted from Wang and Anderson (1982)

Figure 7-1

Finite Difference and Finite Element Representations of an Aquifer Region



Adapted from: Mercer and Faust (1981)

Figure 7-2

Flow Chart to Determine if Modeling is Required

TABLE 7-1

Natural Processes That Affect
Subsurface Contaminant Transport
(after Keely, 1987)

PHYSICAL PROCESSES

- Advection
- Hydrodynamic Dispersion
- Molecular Diffusion
- Density Stratification
- Immiscible Phase Flow
- Fractured Media Flow
- Thermally Driven Flow

CHEMICAL PROCESSES

- Oxidation-Reduction Reactions
- Radionuclide Decay
- Ion-Exchange
- Complexation
- Co-Solvation
- Immiscible Phase Partitioning
- Sorption
- Hydrolysis
- Precipitation/Dissolution

BIOLOGICAL PROCESSES

- Microbial Population Dynamics
- Substrate Utilization
- Biotransformation
- Adaptation
- Co-metabolism