Chapter 5
Computer Modeling of Groundwater Flow

5-1. General

a. Chapter organization. In Chapter 3, an overview of planning and management considerations in performing a groundwater site characterization and modeling study was presented. This chapter provides a technical overview of the theory, development, and use of computer models for simulating groundwater flow. Initially, the criteria to be used in the selection of a computer code are discussed. An overview of the components of a groundwater model is then presented, followed by a discussion on model calibration, execution, and interpretation of results.

b. What is a groundwater model? A groundwater model is a replica of some real-world groundwater system.[1,2,3,4] A groundwater model can be as simple as a construction of saturated sand packed in a glass container or as complex as a three-dimensional mathematical representation requiring solution of hundreds of thousands of equations by a large computer. The term "modeling" refers to the formation of conceptual models and manipulation of modeling software (codes) to represent a site-specific groundwater system. The resulting representation is referred to as a "model" or a "model application." The accuracy of a model is dependent upon the level of understanding of the system the model is to represent. Thus, a complete site investigation and accurate conceptualization of site hydrogeology are necessary precursors to a successful modeling study.

c. Components. As discussed in Chapter 3, basic components of a groundwater modeling project are:

(1) A statement of objectives.

(2) Data describing the physical system.

(3) A simplified conceptual representation of the system.

(4) Data processing and modeling software.

(5) A report containing written and graphical presentations.

d. Protocol. General protocol for performing modeling studies is discussed in Chapter 3, and typically follows a process that includes the following steps:

(1) Determination of modeling objectives.

(2) Data gathering and organization.

(3) Development of a conceptual model.

(4) Numerical code selection.

(5) Assignment of properties and boundary conditions to a grid.

(6) Calibration and sensitivity analysis.

(7) Model execution and interpretation of results.

(8) Reporting.

The following sections in this chapter will focus on steps 4-7; i.e., the technical aspects of developing a computer model of groundwater flow.

5-2. Code Selection

a. Identifying needs. Selecting the appropriate code for a modeling job involves matching modeling

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[1] The International Groundwater Modeling Center defines a model as "a non-unique, simplified, mathematical description of an existing groundwater system, coded in a programming language, together with a quantification of the groundwater system, the code simulates in the form of boundary conditions, system parameters, and system stresses" (U.S. Environmental Protection Agency (USEPA) 1993).

[2] "A model is a simplified description of a physical system" (U.S. Department of Energy 1991).

[3] "A groundwater flow model is an application of a mathematical model to represent a site-specific flow system" (ASTM 1992).

[4] "A mathematical model is a replica of some real world object or system" (Nuclear Regulatory Commission 1992).

needs with the capabilities and controls of available codes. Before selecting a code for use, the modeling objectives, the conceptual model, and project time and cost constraints should be well-defined. Use this information to develop a list of needs. Purchasing a code first, then defining the problem second may cause insurmountable problems. Table 5-1 lists some questions helpful in determining needs and matching these with appropriate codes.

Table 5-1
Determination of Model Needs

Code attributes
What is the general type of problem to be solved (flow in an unconfined aquifer, flow in a fractured confined aquifer, well field design)?
Does the code have the capability to adequately model the hydrologic/geologic features of the site (i.e., wells, rivers, reservoirs, precipitation, watershed runoff, evapotranspiration, variable-density flow, vertical gradients, faults, etc.)?
What are the dimensional capabilities needed (1-D, 2-D Horizontal, 2-D Vertical, quasi 3-D, 3-D)?
What is the best-suited solution method (analytical, finite difference, integrated finite difference, finite element, matrix solver)?
Is a particular mathematical basis needed (empirical vs. mechanistic, deterministic vs. stochastic)?
What grid discretization features are needed?
Will unusual grid size or computational capabilities be required?
What pre- and post-processors are available?
Code administration
Who developed, distributes, and supports the code?
What is the quality of the support?
What is the quality of the user's manual?
What is the cost?
Is the code proprietary?
Is a list of user references available?
Is the code widely used and well verified?

b. Types of codes. Four ways of describing groundwater models are (USEPA 1993):

(1) Objective-based: groundwater supply, well field design, prediction, parameter estimation, and education models.

(2) Process-based: saturated flow, unsaturated flow, contaminant transport, and flow path models.

(3) Physical-system-characteristics based: unconfined aquifer, confined aquifer, porous media, fractured rock, steady-state, time varying, multi-layer, and regional scale models)

(4) Mathematical-based: dimensionality of solution equations, analytical, numerical, empirical, deterministic, and stochastic models.

The above categories are not exclusive. Typically, a model application is labeled using a combination of adjectives from the above categories; for example, a "two-dimensional transient numerical model of groundwater flow in porous media for the prediction of flow paths" is one possible label.

c. Solution methods. Differing solution methods affect the difficulty of use and overall flexibility of modeling software. The three most common solution methods used in groundwater modeling, listed in increasing complexity are: analytical, finite difference, and finite element. Each method solves the governing equation of groundwater flow and storage, but differ in their approaches, assumptions, and applicability to real-world problems.

(1) Analytical methods. Analytical methods use classical mathematical approaches to resolve differential equations into exact solutions. They provide quick results to simple problems. Analytical solutions require assumptions of homogeneity and are limited to one-dimensional and two-dimensional problems. They can provide rough approximations for most problems with little effort. For example, the Thiem equation can be employed to estimate long-term drawdown resulting from pumping in a confined aquifer.

(2) Finite difference methods. Finite difference methods solve the partial-differential equations describing the system by using algebraic equations to approximate the solution at discrete points in a rectangular grid. The grid can be one-, two-, or three-dimensional. The points in the grid, called nodes, represent the average for the surrounding rectangular block (cell). Although adjacent nodes have an effect on the solution process, the value for a particular node is distinct from its neighboring nodes. Grids used in finite difference codes generally require far less set-up time than those of finite element codes, but have less flexibility in individual node placement. Many common codes, such as MODFLOW (McDonald and Harbaugh 1988), use the finite difference solution method.

(3) Finite element methods. Finite element methods differ from finite difference methods in that the area (or volume) between adjacent nodes forms an element over which exact solution values are defined everywhere by means of basis functions. A main practical difference is that finite element codes allow for flexible placement of nodes which can be important in defining irregular boundaries. However, defining a unique location for each finite element node requires a more labor-intensive grid setup than that of finite difference. FEMWATER (Lin et al. 1996) is a common code using the finite element solution method.

d. Code references. Selection of a code ideally requires knowing the capabilities, attributes, and nuances of all available codes, then selecting the most suitable one. There are numerous commercial codes for use in groundwater modeling. Practically, the modeler often lacks up-to-date information on all available codes and lacks sufficient time to sort through code details. An extensive list of codes, their respective characteristics and contact addresses, and an assessment of their usability and reliability is found in the "model information database" of the International Groundwater Modeling Center. A selected listing from that database is found in "Compilation of Groundwater Models" (USEPA 1993). Additional help in selecting a short list of potential codes can be provided by various publications and databases provided by professional organizations and institutes such as the National Groundwater Association, the International Groundwater Modeling Center, and research offices of the CE, USEPA and USGS, among others.

e. Pre- and post-processors.

(1) General. Some pre-processors allow superposition of the grid and the site map, and then allow interactive assignment of boundary conditions, aquifer properties, etc. Post-processors allow the numerical output to be presented as contour maps, raster plots, flow path plots, or line graphs. Choosing a code that does not have, or cannot be easily linked to, pre-and post-processors should be avoided. Hundreds of simulation runs are typically performed for a modeling job, each requiring adjusting input files and interpreting results. Lack of tools to aid in these tasks can cumulatively result in large amounts of additional time spent. An effective link to quality output graphics is critical because many modeling results are best presented pictorially. Systems that include groundwater modeling as just one application in an overall data modeling and representation system are being developed. Such systems reduce overall modeling time by reducing manual data manipulation requirements.

(2) The Department of Defense Groundwater Modeling System. The Department of Defense Groundwater Modeling System (GMS) provides a comprehensive graphical environment for numerical modeling, tools for site characterization, model conceptualization, mesh and grid generation, geostatistics, and sophisticated tools for graphical visualization. Several types of numerical codes are supported by GMS. The current (1996) version of GMS provides a complete interface for the codes MODFLOW, MT3D (a contaminant transport model), and FEMWATER (a finite element model). Many other models will be supported in the future. Tools and features of GMS include the following:

(a) Graphical user interfaces to MODFLOW, MT3D, and FEMWATER groundwater flow and transport codes.

(b) Site characterization using solid modeling of earth masses defined from borehole data.

(c) Surface and terrain modeling using Triangular Irregular Networks.

(d) Automated two- and three-dimensional finite element and finite difference grid generation.

(e) Geostatistical tools for two-dimensional interpolation and three-dimensional interpolation of scattered data, including kriging and natural neighbor interpolation.

(f) Three-dimensional graphics, including contours, vector arrows, shaded images, iso-surfaces, cross sections, and cut-away views.

(g) Animation of steady-state and transient data.

(h) Site maps can be displayed simultaneously with model simulation results.

(i) Intuitive and modular user interface takes advantage of graphical display, and point and click editing.

(j) Available for MS Windows and UNIX platforms.

5-3. Initial Model Development

a. Basic components. After construction of the conceptual model (Chapter 3) and selection of the modeling software, the features of the conceptual model are transferred to an input file that defines the mathematical model. Boundary conditions, grid dimensions and spacing, initial aquifer properties, and time-stepping features are specified according to the particular requirements of the selected code. Input file development can be expedited by use of a pre-processor that allows direct assignment of values to a grid that is superimposed on a site map. At the end of this initial development phase, the model will be ready for calibration.

b. Boundary conditions.

(1) Boundary conditions are constraints imposed on the model grid that express the nature of the physical boundaries of the aquifer being modeled. Boundary conditions have great influence on the computation of flow velocities and heads within the model area. Three types of boundary conditions are commonly used in groundwater flow models:

(a) Specified head. A specified head boundary can be used when expressing the constraints imposed by a lake, a reservoir, or a known phreatic surface. Head data can be measured much easier than flux data, making specified head boundary conditions more desirable for natural features that vary over the length of boundary or vary through time. One caution is that a specified head boundary allows an inexhaustible amount of water flow.

(b) Specified flux. A specified flux boundary expresses the effects of a feature that constrains flow into or out of a boundary or a location where the flux can be estimated. Examples include: zero flux from a subsurface barrier, surface infiltration, leakage across a confining layer, or a “no-flow” boundary chosen to coincide with a groundwater divide or a groundwater flow line so that lateral flux is negligible. Caution should be used in the latter case because natural groundwater divides and “no-flow” lines can move when the aquifer is stressed.

(c) Value-dependent flux. A value-dependent flux allows flux through the boundary according to some external constraint. Examples include infiltration from a pond dependent upon pond levels, and injection of well water dependent upon injection pressure. This type of boundary is used commonly in transient simulations.

(2) Boundary location and orientation. The type of boundary chosen should be fully consistent with the water budget and boundary conditions identified in the conceptual model. Choosing an observable natural feature such as a lake, river, or a groundwater divide as a grid boundary allows the boundary condition to approximate a constraint that can be quantified by measurement (reservoir levels) or reasonable estimate (flux across a groundwater divide). When a natural feature is not available, orienting the boundary to run parallel with a groundwater flow line allows for designation of a boundary with a specified flux of zero. Although the boundaries can be placed anywhere, wise placement reduces uncertainty, thus contributing to more realistic model outcome.

(3) Boundary type variation. Simple models often have uniform conditions for each whole boundary. More detailed models often have boundaries broken into subregions having varying values or differing types of boundary conditions altogether. The type of boundary conditions applied can greatly affect modeling results. A study on boundary condition effects showed that three

groundwater models, the same in all respects except for their boundary conditions, responded very differently to an imposed stress. The study emphasized that when calculated heads match those of the natural system, it does not guarantee that the model boundary conditions match those of the natural system (USGS 1987).

(4) Boundary and system stresses. The location and magnitude of stresses applied to the model affect the appropriate choice of boundary conditions. For example, if a groundwater divide is chosen as a zero-flux boundary condition, the natural boundary and the model boundary may match closely in an unstressed steady state. If, however, an extraction well is placed near this boundary in the computer simulation, the original flow system is no longer being modeled and the original boundary condition and its alignment may need to be changed. A rule of thumb is to avoid placing boundaries close to where stresses will be applied.

(5) Water table boundary. The water table boundary is typically specified three ways: (a) as a dependent variable using the Dupuit assumptions (commonly used in two-dimensional and three-dimensional applications), (b) as a designated no-flow boundary (usually used in three-dimensional and profile applications), or (c) as a dependent variable in an unsaturated/saturated model application. The Dupuit assumptions are: that flow in an unconfined aquifer is horizontal, the head does not change with depth, and that horizontal flow is driven by the water table gradient at all depths. Codes using the Dupuit assumptions allow for treating the water table as the feature to be computed by the model which is often exactly what is desired. The response of the water table to pumping from a well or variations in reservoir stages can be solved with codes using the Dupuit assumptions. Generally speaking, codes using the Dupuit assumptions are more simple and less labor intensive than those requiring the water table to be designated (fixed). Codes requiring an unsaturated/ saturated zone interface have complex and detailed requirements and are generally only used for localized applications because of the detailed definition required.

c. System recharge and withdrawal stresses. Groundwater models are useful in predicting the effects from special recharge and withdrawal stresses, usually injection and extraction wells, that cause a relatively large water exchange in a relatively small area. These analyses can predict general aquifer response to special stresses. However, another method, such as spreadsheet analysis of well drawdown equations, is necessary to simulate the local effect of pumping mainly because node spacing in most site models is typically many times greater than the diameter of the well.

d. Grid design. Model grids discretize the continuous natural system into segments (i.e., cells, elements, blocks) that allow numerical solutions to be calculated. The grid should be superimposed on a map of the area to be modeled. Grid boundaries should be located consistent to the conceptual model and following the guidelines discussed in the boundary condition section. In finite difference modeling, grid nodes lying outside the boundary are often designated as non-computational to minimize computation volume. When designating boundary nodes, the modeler must be aware of whether the modeling software uses a block-centered or mesh-centered convention and place the nodes accordingly. The flux boundary for the mesh-centered nodes is calculated on the line (or plane) directly between the nodes. The flux face is calculated at the midpoint between the nodes when using the block-centered convention. Flexible placement of finite element boundary nodes allows exact placement of nodes along the boundary.

e. Grid resolution and geometry. The following guidelines should be followed when constructing a numerical model grid:

(1) Node spacing. The spacing between nodes, called grid resolution, should be responsive to sharp changes in physical features, temporal conditions, and, numerical stability and overall model size constraints. Generally, node spacing is finer where the dependent variables, usually the hydraulic gradient and flux, are subject to greater change. The areas near extraction wells, infiltration trenches, and confined aquifer flow channels are examples. Finer node placement may also be required where curved surfaces or irregular boundaries are being represented. Where definition of irregular surfaces is required, use of a code not allowing for flexible node placement should be questioned as it could result in a grid with an excessively large number of nodes. Sensitivity to grid resolution should be checked when performing a thorough analysis because differing grid resolutions can affect modeling results.

(2) Selection of model layers. In three-dimensional models, model layers allow for the simulation of flow in separate hydrographic units, leakage between aquifers, and vertical flow gradients. Typically, one model layer is selected for each hydrostratigraphic unit; however, if there are significant vertical head gradients, two or more layers should be used to represent a single hydrostratigraphic unit (Anderson and Woessner 1992).

(3) Avoiding numerical errors. Numerical error and unintended biases in solution of the flow equations can be minimized by avoiding large variations in node spacing and large aspect ratios. The aspect ratio is the maximum dimension of a block or element divided by the minimum dimension. An aspect ratio of one is usually ideal for minimizing numerical errors. As a rule of thumb, aspect ratios up to 10:1 in non-sensitive areas of a grid are usually acceptable and expanding block or element sizes by 1.5 times the adjacent block sizes should be avoided.

(4) Grid sizes. The overall size of the grid (i.e., total number of nodes) should be adequate to define the problem and produce results consistent with modeling objectives, but not so large as to cause excessive run preparation and computation requirements. Several hundred iterations of adjusting the model input, running the model executable code, and interpreting the results are often required in a modeling job. An excessively large grid will expand the time requirements for each iteration, resulting in a cumulatively large impact to the modeling quality or schedule.

f. Initial conditions. Initial conditions refer to the values of the dependent variables defined at the beginning of the simulation. For steady-state models (no time variation), initial conditions need only approximately match the natural system because the solution for each dependent node can be found eventually through repeated iteration. In contrast, transient models (time variation included) require initial conditions closely matching natural conditions at the beginning of the simulation. To do this, it is often necessary to first run a steady-state model, or alternately, run the transient model for a lead-up period of time before beginning the interval of interest. Transient models commonly have boundary conditions that vary as the model simulates an aquifer system response through time. A seasonally fluctuating lake level is an example, and could be simulated using specified head nodes that vary according to some predetermined schedule.

g. Aquifer material properties. Aquifer material properties refer to those aquifer properties, such as hydraulic conductivity and anisotropy, that govern flow rate and flow direction. Table 5-2 presents basic aquifer properties and typical data sources.

Table 5-2
Aquifer Properties and Data Sources

Hydraulic conductivity (pumping tests, slug tests, slug interference tests, grain size analysis, laboratory permeameter tests, tracer tests).
Transmissivity (pumping tests, calculation from hydraulic conductivity).
Porosity (grain size analysis, observation at trenching or outcrop sites, geophysical tests).
Anisotropy (tracer tests, geologic conceptualization and history).
Aquifer storage (pumping tests, geophysical methods).

h. Assignment of aquifer material properties to grid. The aquifer properties previously listed are assigned throughout the model grid by use of a preprocessor or directly into an input file. A simple model may assign uniform hydraulic conductivity in all nodes while complex models may have many different node groups, layers, or zones, each with differing conductivity values. The discretization of zones of homogeneous aquifer properties should be based primarily on site geology. The discretization of zones based on water levels should only be considered in areas where a high quantity (and quality) of data presents compelling physical evidence of distinct hydrogeologic conditions. Geostatistical methods may be employed to distribute the properties to all nodes based on the data known at only a few nodes. However, geostatistics provides a systematic method for distributing the properties and does not account for site geological conditions. The total number of zones of homogeneity should be kept at the minimum required to adequately represent the system within data constraints.

i. Representing uncertainty. The inherent uncertainty in the information describing aquifer properties

should be recognized and preserved throughout the analysis. Most properties should be represented as ranges because of the uncertainty associated with gathering, interpreting, and extrapolating the data to the model. Aquifer properties are usually gross, large-scale representations of properties that are increasingly variable when viewed at increasingly smaller scales. Dealing with uncertainty in model inputs is discussed in Section 5-6 on modeling application.

j. Time-stepping. Time-stepping is the discretizing of the flow equations through time and is used in transient simulations. Like node spacing, time-stepping should be fine enough to define the problem adequately, but not too small to exceed practical computation constraints. Time-stepping should be finer at those times when new stresses are introduced. Changes in boundary conditions usually control the time-step requirement. Initial time-stepping designation should be estimated by experience and refined with a time-stepping sensitivity analysis. Some codes combine time-steps into groups called stress periods.

5-4. Model Calibration and Sensitivity Analysis

a. Calibration defined. Calibration is the process of adjusting model inputs to achieve a desired degree of correspondence between the model simulations and the natural groundwater flow system. A flow model is considered calibrated when it can reproduce, to an acceptable degree, the hydraulic heads and groundwater fluxes of the natural system being modeled. This is accomplished by finding a set of values for the boundary conditions, aquifer properties, and stresses that result in computed heads and fluxes matching their natural counterparts at target locations. In other words, calibration methods solve a problem inversely by iteratively adjusting the unknowns (hydraulic conductivities, certain boundary fluxes, etc.) until the solution matches the knowns (usually the hydraulic heads). Multiple calibrations of the same system are possible using different boundary conditions and aquifer properties. There is not one unique calibration that is "correct" for any model because exact solutions cannot be computed with this multi-variable approach. Furthermore, because model zones of homogeneous aquifer properties should have a strong physical basis, the most accurate model is often not the model which most closely simulates calibration targets. At the end of the calibration process, the model should be ready for use to simulate the flow system.

b. Calibration methods. Methods of calibrating can be grouped into two categories: manual trial-and-error calibration and automated calibration. The state of the practice is that most modeling is performed by trial and error while automated methods are becoming increasingly usable and accepted. The method is code-dependant. Advances in modeling software allowing for greater use of automated calibration are expected.

(1) Manual trial and error. This method of calibration is labor-intensive. The modeler makes successive cycles involving interpreting prior results to determine where inputs need adjustment, making speculative adjustments to the input code, re-running the model and output software, and then comparing the computed results to the natural system. Typically, hundreds of iterations are made before an acceptable calibration is achieved, the specific number depending on model complexity, experience of the modeler, and the acceptableness criteria applied. Typically, the inputs being adjusted are hydraulic conductivity (or transmissivity), storage, leakage across a confining layer used as a boundary, flux to and from a surface water body, and designation of boundary conditions. A typical manual trial-and-error calibration process includes the following steps:

(a) Complete initial model development and assignment of properties as outlined in this chapter.

(b) Identify the parameters to be adjusted during calibration and the appropriate range for each. These are determined from the initial sensitivity analysis and from the conceptual model.

(c) Identify the locations and values for the target points forming the calibration set. Groundwater flow models are usually calibrated to a set of observed potentiometric head levels.

(d) Iteratively run the modeling software and adjust input parameters until an acceptable match between observed and calculated values at the target points is achieved. If the model is being calibrated to a set of observed head values, the computed and estimated boundary fluxes must also be compared.

(e) Repeat steps (c) and (d) for different calibration conditions if desired. For example, a model can be calibrated to the seasonal low and seasonal high calibration conditions or to conditions where the aquifer is stressed by pumping or injection.

(2) Automated calibration. This method utilizes an objective function, such as minimization of the sum of the squared differences between observed and computed heads (residuals), to govern automatic iterative adjustment of values that would otherwise be adjusted manually. Automated codes do this in a systematic fashion and typically require constraints on sets of input values in the form of probability functions, conditional bounds, or weighted values. These constraints require the modeler to better define the uncertainty and variation within parameters, such as hydraulic conductivity, before code execution begins. Particular requirements for automated calibration codes vary.

(3) Comparison of calibration methods. Automated calibration methods have some potential advantages over trial-and-error methods. They can provide a systematic approach to calibration, allowing for efficiencies within individual modeling jobs and a basis for comparison between different modeling jobs. Statistical measurements are available from some automated approaches that are not usually performed in trial-and-error approaches. And finally, practitioners report that, because less time was spent on manual iteration, more time was available to refine the calibration and explore model sensitivity to various calibration options.

c. Matching computed values with target values. A key to calibration is the comparison of computed values, usually the computed heads, with observed values, often called "target values," to determine the appropriateness of the calibration. Questions to be considered when compiling a set of target values include the following:

(1) Do the target values reflect a steady-state or transient condition?

(2) Are there effects from local anomalies?

(3) Are the wells screened comparably?

(4) Are the measurement errors acceptable?

These questions can usually be answered by having a complete conceptual model and observing the changes to the set of target values over time.

d. Types of comparisons.

(1) Spatial graphic comparisons. This method often uses superimposed contoured water table surfaces or raster plots to show locations and magnitude of the differences between computed and observed values (residuals). These methods provide the modeler with an understanding of spatial variation of the residuals and can be key to selecting where further input parameter adjustments are required.

(2) Tabular comparison at target nodes. This method provides a quantifiable comparison of values point by point.

(3) Lumped-sum comparison. These methods lump residual measurements into single values and often take the form of: (a) mean error of the residuals, (b) absolute mean error to the residuals, and (c) root-mean-squared error of the residuals. Using the root-mean-squared error method provides a commonly used overall comparison.

e. Calibration cautions. Successful calibration to one model component does not guarantee a sound model.

(1) Head calibrations and boundary conditions. When model head results match observed head results, the groundwater flow system is not necessarily simulated accurately. As discussed in the "Boundary Conditions" section, research shows that models differing only by their boundary conditions can be calibrated to the same hydraulic head set, yet perform differently when stressed. Similarly, models that differ only by magnitude of hydraulic conductivity values can be calibrated to the same water table head set, yet produce differing flow velocities and boundary fluxes. These potential difficulties can be overcome to some degree by development of a sound conceptual model and ensuring the mathematical model appropriately represents key conceptual components. Estimated fluxes should be compared with calculated fluxes for any calibration using hydraulic heads as target values. Boundary conditions play an important role in soundness of modeling.

(2) Experience required. Model calibration requires extensive knowledge of the natural groundwater system being modeled. Understanding how to best achieve an adequate calibration and when the match between results is "good enough" depends on modeling objectives and expectations of the customers. Freyberg (1988) documents a study where nine groups, using the same model and input data, individually calibrated the model and produced widely varied final results. "The group achieving the best prediction chose to zone the conductivity field into a relatively few homogenous regions, while the group producing the worst prediction chose to 'tweak' the conductivity field grid block by grid block to achieve a good (in fact, the best) local fit to the observed data." This study showed that an apparently "good" calibration does not necessarily result in accurate predictive results for other simulations.

f. Sensitivity analysis defined. A sensitivity analysis is a quantitative evaluation of the influence on model outputs from variation of model inputs. A sensitivity analysis identifies those parameters most influential in determining the accuracy and precision of model predictions (USEPA 1992). During sensitivity analysis, numerous model runs are performed, each having only one parameter varied by some specified percentage. Both positive and negative variance is tested.

g. Use of sensitivity analyses. Sensitivity analyses can be used to aid in model construction by identifying inputs requiring more definition. For example, the sensitivity analysis may show that existing hydraulic conductivity data ranges so widely that additional pumping tests are needed to obtain the desired level of accuracy in modeling results. Sensitivity analyses also aid in interpreting results. For example, uncertainty about the head values at a boundary may not be a concern if the analysis shows that output of interest is insensitive to these head values. Typically the analysis will show that sensitivity of groundwater flow to variation in hydraulic conductivity is relatively high.

h. Level of effort. Commonly, a small-scale analysis is performed during early model calibration, as a calibration aid; then a more rigorous analysis is performed after calibration as an indicator of model performance. If, for example, the results from a sensitivity analysis show that computed velocities vary ± 20 percent due to the reasonably expected range of site hydraulic conductivities, then interpretation of final model results should reflect this.

5-5. History Matching

Following calibration and sensitivity analyses, the model application can be tested with the concept of history matching. The concept of history matching is that a model's predictive capability can be shown to reside within acceptable limits by comparing model predictions with a data set independent of the calibration data. If the comparison is unfavorable, the model needs further calibration. If the comparison is favorable, it gives weight to the argument that the model application can be used for prediction with a reasonable assurance of accuracy. This assurance does not, however, extend to conditions other than those tested and thus does not account for unforeseen stresses. History matching shows how the model application can simulate past conditions. It does not necessarily indicate accuracy for predictive simulations.

5-6. Model Execution and Interpretation of Results

a. Model execution. After successfully performing the calibration and sensitivity analysis, the model application is ready for use in performing simulations. This step usually takes less time than the calibration step. Model output is usually produced in the form of hydraulic heads and flow vectors at grid nodes. From these, head contour maps, flow field vector maps, groundwater pathline maps, and water balance calculations can be made using post processors. Some combination of these simulation results can be used to answer the questions posed by the modeling objectives.

b. Dealing with uncertainty. One key issue is how to constrain the modeling runs to account for uncertainty while still meeting the modeling objectives. This can be accomplished by using one of the following approaches:

(1) Best estimate. Producing "best estimate" results by using the most representative input values usually provides a useful indicator of groundwater velocities, heads, and fluxes. However, single value modeling results do not, by themselves, give much assurance of accuracy.

(2) Worst case. One possible modeling objective is to determine if a certain groundwater level or flow rate may arise given the most unfavorable conditions possibly expected. In this case, the model is calibrated using the best estimates from the ranges of input values, but simulations are performed using input values from the most unfavorable end of the input ranges. For example, field estimates for transmissivities are identified at 500-800 m^3/d-m. If model simulations predict that a well field design will meet its production goals even when using transmissivities as low as 400 m^3/d-m, this gives some assurance that the design is adequate.

(3) Best estimate with sensitivity analysis adjustment. Best estimate results can be coupled with the results from the sensitivity analysis to provide a range of expected aquifer performance. For example, if modeling objectives were to predict whether head fluctuations at a location could exceed 5 m, and, if the best estimate results plus additional adjustment from the sensitivity analysis results predict only a total of 2 m expected fluctuation, then further analysis may not be warranted.

(4) Bracketed ranges. In this case, two or more calibrations of the model are made. Each uses a different set of values for key input parameters. The results should bracket the expected possible range of results. For example, if field data defined a dominant hydrogeologic unit at a site, but the only two pumping tests for this unit produced differing estimates of its hydraulic conductivity, a model could be calibrated twice using the two different estimates. These two calibrations would differ in boundary flux and flow velocities which should be checked against observed or estimated values. Bracketing gives those interpreting modeling results a greater understanding of how overall model performance varies according to input uncertainty.

(5) Using uncertainty distributions. Various methods, such as inverse modeling and Monte Carlo analysis, can be used to more fully analyze the effects of uncertainty on modeling results. Usually these methods require the modeler to bound the range of uncertainty or define a probability distribution for the associated variable. Results are returned in bounded or distribution form. The level of effort and computation time required for these types of analyses are much greater than those of earlier described approaches. Advances in software are expected to increase the usability of these approaches in the future.

5-7. Post Audit

A post audit is similar to history matching described in Section 5-5, but differs in that it assesses the accuracy of past predictions compared with data gathered in the interim period (usually over a long period of time). Post audits usually provide insights into model improvements that can be made and weaknesses in making modeling assumptions. Anderson and Woessner (1992) report on four post audits reported in widely available literature none of which accurately predicted the future. They concluded that inaccurate predictions were based on errors in the conceptual models and also on failure to use appropriate values for assumed future stresses. When modeling is viewed as an iterative process continuing over long periods of time, then modeling performed today will provide a basis for future modeling which will be improved by larger data sets and improved technology.