United States Environmental Protection Agency
Office of Research and Development
Office of Solid Waste and Emergency Response
EPA/540/S-92/005
April 1992

Ground Water Issue

Fundamentals of Ground-Water Modeling

Jacob Bear[a], Milovan S. Beljin[b], and Randall R. Ross[c]

Ground-water flow and contaminant transport modeling has been used at many hazardous waste sites with varying degrees of success. Models may be used throughout all phases of the site investigation and remediation processes. The ability to reliably predict the rate and direction of ground-water flow and contaminant transport is critical in planning and implementing ground-water remediations. This paper presents an overview of the essential components of ground-water flow and contaminant transport modeling in saturated porous media. While fractured rocks and fractured porous rocks may behave like porous media with respect to many flow and contaminant transport phenomena, they require a separate discussion and are not included in this paper. Similarly, the special features of flow and contaminant transport in the unsaturated zone are also not included. This paper was prepared for an audience with some technical background and a basic working knowledge of ground-water flow and contaminant transport processes. A suggested format for ground-water modeling reports and a selected bibliography are included as appendices A and B, respectively.

For further information, contact David Burden (FTS 700-743-2294), Randall Ross (FTS 700-743-2355), or Joe Williams (FTS 700-743-2312) at (405) 332-8800.

Modeling as a Management Tool

The management of any system means making decisions aimed at achieving the system's goals, without violating specified technical and nontechnical constraints imposed on it. In a ground-water system, management decisions may be related to rates and location of pumping and artificial recharge, changes in water quality, location and rates of pumping in pump-and-treat operations, etc. Management's objective function should be to evaluate the time and cost necessary to achieve remediation goals. Management decisions are aimed at minimizing this cost while maximizing the benefits to be derived from operating the system.

The value of management's objective function (e.g., minimize cost and maximize effectiveness of remediation) usually depends on both the values of the decision variables (e.g., areal and temporal distributions of pumpage) and on the response of the aquifer system to the implementation of these decisions. Constraints are expressed in terms of future values of state variables of the considered ground-water system, such as water table elevations and concentrations of specific contaminants in the water. Typical constraints may be that the concentration of a certain contaminant should not exceed a specified value, or that the water level at a certain location should not drop below specified levels. Only by comparing predicted values with specified constraints can decision makers conclude whether or not a specific constraint has been violated.

An essential part of a good decision-making process is that the response of a system to the implementation of contemplated decisions must be known *before* they are implemented.

In the management of a ground-water system in which decisions must be made with respect to both water quality and water quantity, a tool is needed to provide the decision maker with information about the future response of the system to the effects of management decisions. Depending on the nature of

[a] *Technion - Israel Institute of Technology*
[b] *University of Cincinnati*
[c] *U.S. EPA, Robert S. Kerr Environmental Research Laboratory*

COMMUNICATION • TRAINING • TECHNOLOGY SUPPORT
Technology Support Project

Superfund Technology Support Center for Ground Water

Robert S. Kerr Environmental Research Laboratory
Ada, Oklahoma

Technology Innovation Office
Office of Solid Waste and Emergency Response, US EPA, Washington, DC

Walter W. Kovalick, Jr., Ph.D.
Director

the management problem, decision variables, objective functions, and constraints, the response may take the form of future spatial distributions of contaminant concentrations, water levels, etc. This tool is the *model*.

Examples of potential model applications include:

- Design and/or evaluation of pump-and-treat systems
- Design and/or evaluation of hydraulic containment systems
- Evaluation of physical containment systems (e.g., slurry walls)
- Analysis of "no action" alternatives
- Evaluation of past migration patterns of contaminants
- Assessment of attenuation/transformation processes
- Evaluation of the impact of nonaqueous phase liquids (NAPL) on remediation activities (dissolution studies)

What Is a Ground-Water Model?

A model may be defined as a simplified version of a real-world system (here, a ground-water system) that approximately simulates the relevant excitation-response relations of the real-world system. Since real-world systems are very complex, there is a need for simplification in making planning and management decisions. The simplification is introduced as a set of assumptions which expresses the nature of the system and those features of its behavior that are relevant to the problem under investigation. These assumptions will relate, among other factors, to the geometry of the investigated domain, the way various heterogeneities will be smoothed out, the nature of the porous medium (e.g., its homogeneity, isotropy), the properties of the fluid (or fluids) involved, and the type of flow regime under investigation. Because a model is a simplified version of a real-world system, no model is unique to a given ground-water system. Different sets of simplifying assumptions will result in different models, each approximating the investigated ground-water system in a different way. The first step in the modeling process is the construction of a *conceptual model* consisting of a set of assumptions that *verbally* describe the system's composition, the transport processes that take place in it, the mechanisms that govern them, and the relevant medium properties. This is envisioned or approximated by the modeler for the purpose of constructing a model intended to provide information for a specific problem.

Content of a Conceptual Model

The assumptions that constitute a conceptual model should relate to such items as:

- the geometry of the boundaries of the investigated aquifer domain;
- the kind of solid matrix comprising the aquifer (with reference to its homogeneity, isotropy, etc.);
- the mode of flow in the aquifer (e.g., one-dimensional, two-dimensional horizontal, or three-dimensional);
- the flow regime (laminar or nonlaminar);
- the properties of the water (with reference to its homogeneity, compressibility, effect of dissolved solids and/or temperature on density and viscosity, etc.);
- the presence of assumed sharp fluid-fluid boundaries, such as a phreatic surface;
- the relevant state variables and the area, or volume, over which the averages of such variables are taken;
- sources and sinks of water and of relevant contaminants, within the domain and on its boundaries (with reference to their approximation as point sinks and sources, or distributed sources);
- initial conditions within the considered domain; and
- the conditions on the boundaries of the considered domain that express the interactions with its surrounding environment.

Selecting the appropriate conceptual model for a given problem is one of the most important steps in the modeling process. Oversimplification may lead to a model that lacks the required information, while undersimplification may result in a costly model, or in the lack of data required for *model calibration* and *parameter estimation*, or both. It is, therefore, important that all features relevant to a considered problem be included in the conceptual model and that irrelevant ones be excluded.

The selection of an appropriate conceptual model and the degree of simplification in any particular case depends on:

- the objectives of the management problem;
- the available resources;
- the available field data;
- the legal and regulatory framework applying to the situation.

The objectives dictate which features of the investigated problem should be represented in the model, and to what degree of accuracy. In some cases averaged water levels taken over large areas may be satisfactory, while in others water levels at specified points may be necessary. Natural recharge may be introduced as monthly, seasonal or annual averages. Pumping may be assumed to be uniformly distributed over large areas, or it may be represented as point sinks. Obviously, a more detailed model is more costly and requires more skilled manpower, more sophisticated codes and larger computers. It is important to select the appropriate degree of simplification in each case.

Selection of the appropriate conceptual model for a given problem is not necessarily a conclusive activity at the initial stage of the investigations. Instead, modeling should be considered as a continuous activity in which assumptions are reexamined, added, deleted and modified as the investigations continue. It is important to emphasize that the availability of field data required for model calibration and parameter estimation dictates the type of conceptual model to be selected and the degree of approximation involved.

The next step in the modeling process is to express the (verbal) conceptual model in the form of a *mathematical model*. The solution of the mathematical model yields the required predictions of the real-world system's behavior in response to various sources and/or sinks.

Most models express nothing but a balance of the considered extensive quantity (e.g., mass of water or mass of solute). In the *continuum approach*, the balance equations are written "at a point within the domain," and should be interpreted to mean "per unit area, or volume, as the case may be, in the vicinity of the point." Under such conditions, the balance takes the form of a partial differential equation. Each term in that equation expresses a quantity added per unit area or per unit volume, and per unit time. Often, a number of extensive quantities of interest are transported simultaneously; for example, mass of a number of fluid phases with each phase containing more than one relevant species. The mathematical model will then contain a balance equation for each extensive quantity.

Content of a Mathematical Model

The complete statement of a mathematical model consists of the following items:

- a definition of the geometry of the considered domain and its boundaries;
- an equation (or equations) that expresses the balance of the considered extensive quantity (or quantities);
- flux equations that relate the flux(es) of the considered extensive quantity(ies) to the relevant state variables of the problem;
- constitutive equations that define the behavior of the fluids and solids involved;
- an equation (or equations) that expresses initial conditions that describe the known state of the considered system at some initial time; and
- an equation (or equations) that defines boundary conditions that describe the interaction of the considered domain with its environment.

All the equations must be expressed in terms of the dependent variables selected for the problem. The selection of the appropriate variables to be used in a particular case depends on the available data. The number of equations included in the model must be equal to the number of dependent variables. The boundary conditions should be such that they enable a unique, stable solution.

The most general boundary condition for any extensive quantity states that the difference in the normal component of the total flux of that quantity, on both sides of the boundary, is equal to the strength of the source of that quantity. If a source does not exist, the statement reduces to an equality of the normal component of the total flux on both sides of the boundary. In such equalities, the information related to the external side must be known (Bear and Verruijt, 1987). It is obtained from field measurements or on the basis of past experience.

The mathematical model contains the same information as the conceptual one, but expressed as a set of equations which are amenable to analytical and numerical solutions. Many mathematical models have been proposed and published by researchers and practitioners (see Appendix B). They cover most cases of flow and contaminant transport in aquifers encountered by hydrologists and water resource managers. Nevertheless, it is important to understand the procedure of model development.

The following section introduces three fundamental assumptions, or items, in conceptual models that are always made when modeling ground-water flow and contaminant transport and fate.

The Porous Medium as a Continuum

A *porous medium* is a continuum that replaces the real, complex system of solids and voids, filled with one or more fluids, that comprise the aquifer. Inability to model and solve problems of water flow and contaminant transport within the void space is due to the lack of detailed data on its configuration. Even if problems could be described and solved at the *microscopic* level, measurements cannot be taken at that level (i.e., at a point within the void space), in order to validate the model. To circumvent this difficulty, the porous medium domain is visualized as a continuum with fluid or solid matrix variables defined at *every* point. Not only is the porous medium domain as a whole visualized as a continuum, but each of the phases and components within it is also visualized as a continuum, with all continua overlapping each other within the domain.

The passage from the microscopic description of transport phenomena to a macroscopic one is achieved by introducing the concept of a *representative elementary volume* (REV) of the porous medium domain. The main characteristic of an REV is that the averages of fluid and solid properties taken over it are independent of its size. To conform to this definition, the REV should be much larger than the microscopic scale of heterogeneity associated with the presence of solid and void spaces, and much smaller than the size of the considered domain. With this concept of an REV in mind, a porous medium domain can be defined as a portion of space occupied by a number of phases: a solid phase (i.e., the solid matrix), and one or more fluid phases, for which an REV can be found.

Thus, a macroscopic value at a point within a porous medium domain is interpreted as the average of that variable taken over the REV centered at that point. By averaging a variable over all points within a porous medium domain, a continuous field of that variable is obtained.

By representing the actual porous medium as a continuum, the need to know the detailed microscopic configuration of the void space is circumvented. However, at the macroscopic level, the complex geometry of the void-solid interface is replaced by various solid matrix coefficients, such as porosity, permeability and dispersivity. Thus, a coefficient that appears in a macroscopic model represents the relevant effect of the microscopic void-space configuration.

In practice, all models describing ground-water flow and contaminant transport are written at the continuum, or macroscopic level. They are obtained by averaging the corresponding microscopic models over the REV. This means that one must start by understanding phenomena that occur at the microscopic level, (e.g., on the boundary between adjacent phases) before deriving the macroscopic model. For most models of practical interest, this has already been done and published.

Horizontal Two-Dimensional Modeling

A second fundamental approximation often employed in dealing with regional problems of flow and contaminant transport is that ground-water flow is essentially horizontal. The term “regional” is used here to indicate a relatively large aquifer domain. Typically, the horizontal dimension may be from tens to hundreds of kilometers with a thickness of tens to hundreds of meters.

In principle, ground-water flow and contaminant transport in a porous medium domain are three-dimensional. However, when considering regional problems, one should note that because of the ratio of aquifer thickness to horizontal length, the flow in the aquifer is practically horizontal. This observation also remains valid when small changes exist in the thickness of a confined aquifer, or in the saturated thickness of an unconfined aquifer. On the basis of this observation, the assumption that ground-water flow is essentially horizontal is often made and included in the conceptual model. This leads to an aquifer flow model written in horizontal two dimensions only. Formally, the two-dimensional horizontal flow model is obtained by integrating the corresponding three-dimensional variable over the aquifer's thickness. This procedure is known as the *hydraulic approach*. The two-dimensional horizontal flow model is written in terms of variables which are averaged over the vertical thickness of the aquifer and thus are a function of the horizontal coordinates only.

In the process of transforming a three-dimensional problem into a two-dimensional one, new aquifer transport and storage coefficients (e.g., aquifer transmissivity and storativity) appear. In addition to the advantage of having to solve a two-dimensional rather than a three-dimensional mathematical model, fewer field observations may be required for the determination of these coefficients.

Whenever justified on the basis of the geometry (i.e., thickness versus horizontal length) and the flow pattern, the assumption of essentially horizontal flow greatly simplifies the mathematical analysis of the flow in an aquifer. The error introduced by this assumption is small in most cases of practical interest.

The assumption of horizontal flow fails in regions where the flow has a large vertical component (e.g., in the vicinity of springs, rivers or partially penetrating wells). However, even in these cases, at some distance from the source or sink, the assumption of horizontal flow is valid again. As a general rule, one may assume horizontal flow at distances larger than 1.5 to 2 times the thickness of the aquifer in that vicinity (Bear, 1979). At smaller distances the flow is three-dimensional and should be treated as such.

The assumption of horizontal flow is also applicable to leaky aquifers. When the hydraulic conductivity of the aquifer is much larger than that of the semipermeable layer, and the aquifer thickness is much larger than the thickness of the aquitard, it follows from the law of refraction of streamlines ("tangent law") that the flow in the aquifer is essentially horizontal, while it is practically vertical in the aquitards (de Marsily, 1986).

When considering contaminant transport in aquifers, the model user must be cautious in attempting to utilize a two-dimensional model, because in most cases the hydraulic approach is not justified . The contaminant may be transported through only a small fraction of the aquifer's thickness. In addition, velocities in different strata may vary appreciably in heterogeneous aquifers, resulting in a marked difference in the rates of advance and spreading of a contaminant.

Momentum Balance

The third concept relates to the fluid's momentum balance. In the continuum approach, subject to certain simplifying assumptions included in the conceptual model, the momentum balance equation reduces to the linear motion equation known as *Darcy's law*. This equation is used as a flux equation for fluid flow in a porous medium domain. With certain modifications, it is also applicable to multiphase flows (e.g., air-water flow in the unsaturated zone).

Major Balance Equations

The following examples of major balance equations constitute the core of models that describe flow and contaminant transport in porous medium domains. A number of simplifying assumptions must be stated before any of these equations can be written. Although these assumptions are not listed here, they must be included in the conceptual model of the respective cases.

Mass balance for 3-D saturated flow in a porous medium domain:

$$S_o \frac{\varphi}{t} = \cdot \, (\mathbf{K} \cdot \quad \varphi) \,, \qquad (1)$$

where S_o = specific storativity of porous medium
φ = piezometric head
$\mathbf{K}$ = hydraulic conductivity tensor

The specific storativity, S_o , is defined as the volume of water added to storage in a unit volume of porous medium, per unit rise of piezometric head. Hence, the left side of equation (1) expresses the volume of water added to storage in the porous medium domain per unit volume of porous medium per unit time. The divergence of a flux vector, $\mathbf{q}$, written mathematically as $\cdot \; \mathbf{q}$, expresses the excess of outflow over inflow per unit volume of porous medium, per unit time. The flux q is expressed by Darcy's law,

$$\mathbf{q} = -\mathbf{K} \cdot \quad \varphi$$

Note that in equation (1), the operators (scalar) (to be read as "gradient of the scalar"), and • (vector) (to be read as the "divergence of the vector"), are in the three-dimensional space. The variable to be solved is $\varphi\,(x,y,z,t)$.

Thus, equation (1) states that the excess of inflow over outflow of water in a unit volume of porous medium, per unit time, at a point, is equal to the rate at which water volume is being stored, where storage is due to fluid and solid matrix compressibilities.

Mass balance for 2-D saturated flow in a confined aquifer:

$$S \quad \frac{\varphi}{t} = \cdot \, (\mathbf{T} \cdot \quad \varphi) - P\,(x,y,t) + R\,(x,y,t) \qquad (2)$$

where S = aquifer storativity
φ = piezometric head
$\mathbf{T}$ = aquifer transmissivity tensor
$P\,(x,y,t)$ = rate of pumping (per unit area of aquifer)
$R\,(x,y,t)$ = rate of recharge (per unit area of aquifer)

The storativity, S, is defined as the volume of water added to storage in a unit area of aquifer, per unit rise of piezometric head. Hence, the left side of equation (2) expresses the volume of water added to storage in the aquifer, per unit area per unit time. The divergence of a flux vector,(= $-\mathbf{T} \bullet \varphi$), expresses the excess of outflow over inflow per unit area, per unit time. Note that here, the two operators are in the two-dimensional horizontal coordinates, and the variable to be solved is $\varphi(x,y,t)$.

Thus, equation (2) states that the excess of inflow over outflow of water in a unit area of an aquifer, per unit time, at a point, is equal to the rate at which water volume is being stored, where storage is due to fluid and solid matrix compressibilities.

Mass balance for a solute in 3-D saturated flow:

The left side of equation (3) expresses the mass of the conservative solute added to storage per unit volume of porous medium per unit time (e.g., it does not adsorb, decay or interact with the solid matrix).

$$\frac{\phi\, c}{t} = - \quad \bullet (c\,\mathbf{q} + \phi\,\mathbf{J} + \phi\,\mathbf{J}) + \Gamma \qquad (3)$$

where
- c = concentration of considered solute
- ϕ = porosity of porous medium
- $\mathbf{q}$ = specific discharge of water (= volume of water passing through a unit area of porous medium per unit time)
- $\mathbf{J}^*$ = dispersive flux of solute (per unit area of fluid)
- $\mathbf{J}$ = diffusive flux of solute (per unit area of fluid)
- Γ = strength of solute source (added quantity per unit volume of porous medium per unit time)

The first term on the right side of equation (3) (to be read as "minus divergence of the total flux of the solute"), expresses the excess of the solute's inflow over outflow, per unit volume of porous medium, per unit time. This total flux is made up of an advective flux with the fluid, a dispersive flux and a diffusive flux. The second term on the right side of equation (3) expresses the added mass by various sources.

The dispersive and diffusive fluxes appearing in equation (3) must be expressed in terms of the concentration, *c*, which serves as the variable to be solved in this equation. For example,

$$\mathbf{J} = -\mathcal{D}^* \bullet\ c, \qquad \mathbf{J}^* = -\mathbf{D} \bullet\ c,$$

where
- $\mathbf{D}$ = coefficient of dispersion
- $\mathcal{D}^*$ = coefficient of molecular diffusion in a porous medium

Model Coefficients and Their Estimation

In passing from the microscopic level of describing transport to the macroscopic level, various coefficients of transport and storage are introduced. The permeability of a porous medium, aquifer transmissivity, aquifer storativity, and porous medium dispersivity, may serve as examples of such coefficients. Permeability and dispersivity are examples of coefficients that express the macroscopic effects of microscopic configuration of the solid-fluid interfaces of a porous medium. They are introduced in the passage from the microscopic level of description to the macroscopic, continuum, level. The coefficients of aquifer storativity and transmissivity are introduced by the further averaging of the three-dimensional macroscopic model over the thickness of an aquifer in order to obtain a two-dimensional model. All these coefficients are coefficients of the models, and therefore, in spite of the similarity in their names in different models, their interpretation and actual values may differ from one model to the next.

This point can be illustrated by the following example. To obtain the drawdown in a pumping well and in its vicinity, one employs a conceptual model that assumes radially converging flow to an infinitesimally small well in a homogeneous, isotropic aquifer of constant thickness and of infinite areal extent. The same model is used to obtain the aquifer's storativity and transmissivity by conducting an aquifer pumping test and solving the model's equation for these coefficients. It is common practice to refer to these coefficients as the aquifer's coefficients and not as coefficients of the aquifer's model. However, it is important to realize that the coefficients thus derived actually correspond to that particular model. These coefficients should not be employed in a model that describes the flow in a finite heterogeneous aquifer with variable thickness and with non-radial flow in the vicinity of the well. Sometimes, however, there is no choice because this is the only information available. Then, the information must be used, keeping in mind that when coefficients are derived by employing one model in another model for a given domain, the magnitude of the error will depend on the differences between the two models. In principle, in order to employ a particular model, the values of the coefficients appearing in it should be determined using some parameter identification technique for that particular model.

Obviously, no model can be employed in any specified domain unless the numerical values of all the coefficients appearing in it are known. Estimates of natural recharge and a priori location and type of boundaries may be included in the list of model coefficients and parameters to be identified. The activity of identifying these model coefficients is often referred to as the *identification problem*.

In principle, the only way to obtain the values of the coefficients for a considered model is to start by investigating the real-world aquifer system to find a period (or periods) in the past for which information is available on (*i*) initial conditions of the system; (*ii*) excitations of the system, as in the form of pumping and artificial recharge (quality and quantity), natural recharge introduction of contaminants, or changes in boundary conditions, and (*iii*) observations of the response of the system, as in the form of temporal and spatial distributions of water levels and solute concentrations. If such a period (or periods) can be found, one can (*i*) impose the known initial conditions on the model, (*ii*) excite the model by the known excitations of the real system, and (*iii*) derive the response of the model to these excitations. Obviously, in order to derive the model's response, one has to assume some trial values for the coefficients and compare the response observed in the real system with that predicted by the model. The sought values of the coefficients are those that will make the two sets of values of state variables identical. However, because the model is only an approximation of the real system, one should never expect these two sets of values to be identical. Instead, the “best fit” between them must be sought according to some criterion. Various techniques exist for determining the “best” or “optimal” values of these coefficients (i.e., values that will make the predicted values and the measured ones sufficiently close to each other). Obviously, the values of the coefficients eventually accepted as “best” for the model depend on the criteria selected for “goodness of fit” between the observed and predicted values of the relevant state variables. These, in turn, depend on the objective of the modeling.

Some techniques use the basic trial-and-error method described above, while others employ more sophisticated optimization methods. In some methods, *a priori* estimates of the coefficients, as well as information about lower and upper bounds, are introduced. In addition to the question of selecting the appropriate criteria, there remains the question of the conditions under which the identification problem, also called the inverse problem, will result in a unique solution.

As stressed above, no model can be used for predicting the behavior of a system unless the numerical values of its parameters have been determined by some identification procedure. This requires that data be obtained by field measurements. However, even without such data, certain important questions about the suitability of the model can be studied. Sensitivity analysis enables the modeler to investigate whether a certain percentage change in a parameter has any real significance, that is whether it is a dominant parameter or not. The major point to be established from a sensitivity analysis is the relative sensitivity of the model predictions to changes in the values of the model parameters within the estimated range of such changes.

A successful model application requires appropriate site characterization and expert insight into the modeling process. Figure 1 illustrates a simple diagram of a model application process. Each phase of the process may consist of various steps; often, results from one step are used as feedback in previous steps, resulting in an iterative procedure (van der Heijde et al., 1989).

Methods of Solution

Once a well-posed model for a given problem has been constructed, including the numerical values of all the coefficients that appear in the model, it must be solved for any given set of excitations (i.e., initial and boundary conditions,

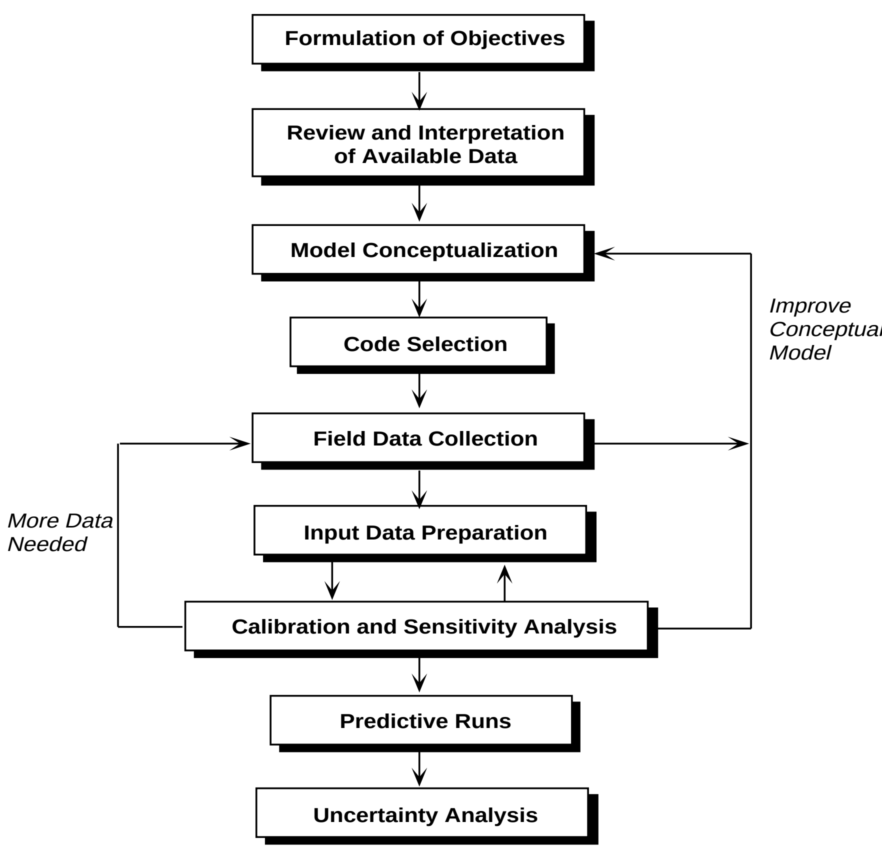

Figure 1. Model Application Process.

sources and sinks). The preferable method of solution is the analytical one, as once such a solution is derived, it can be used for a variety of cases (e.g., different values of coefficients, different pumping rates, etc). However, for most cases of practical interest, this method of solution is not possible due to the irregularity of the domain's shape, the heterogeneity of the domain with respect to various coefficients, and various nonlinearities. Instead, numerical models are employed.

Although a numerical model is derived from the mathematical model, a numerical model of a given problem need not necessarily be considered as the numerical method of solution, but as a model of the problem in its own right. By adding assumptions to the conceptual model of the given problem (e.g., assumptions related to time and space discretization) a new conceptual model is obtained which, in turn, leads to the numerical model of the given problem. Such a model represents a different approximate version of the real system.

Even those who consider a numerical model as a model in its own right very often verify it by comparing the model results with those obtained by an analytical solution of the corresponding mathematical model (for relatively simple cases for which such solutions can be derived). One of the main reasons for such a verification is the need to eliminate errors resulting from the numerical approximations alone. Until the early 1970s, physical (e.g., sand box) and analog (e.g., electrical) laboratory models were used as practical tools for solving the mathematical models that described ground-water flow problems. With the introduction of computers and their application in the solution of numerical models, physical and analog models have become cumbersome as tools for simulating ground-water regimes. However, laboratory experiments in soil columns are still needed when new phenomena are being investigated and to validate new models (i.e., to examine whether certain assumptions that underlie the model are valid).

Analytical Models

During the early phase of a ground-water contamination study, analytical models offer an inexpensive way to evaluate the physical characteristics of a ground-water system. Such models enable investigators to conduct a rapid preliminary analysis of ground-water contamination and to perform sensitivity analysis. A number of simplifying assumptions regarding the ground-water system are necessary to obtain an analytical solution. Although these assumptions do not necessarily dictate that analytical models cannot be used in "real-life" situations, they do require sound professional judgment and experience in their application to field situations. Nonetheless, it is also true that in many field situations few data are available; hence, complex numerical models are often of limited use. When sufficient data have been collected, however, numerical models may be used for predictive evaluation and decision assessment. This can be done during the later phase of the study. Analytical models should be viewed as a useful complement to numerical models.

For more information on analytical solutions, the reader is referred to Bear (1979), van Genuchten and Alves (1982), and Walton (1989).

Numerical Models

Once the conceptual model is translated into a mathematical model in the form of governing equations, with associated boundary and initial conditions, a solution can be obtained by transforming it into a numerical model and writing a computer program (code) for solving it using a digital computer.

Depending on the numerical technique(s) employed in solving the mathematical model, there exist several types of numerical models:

- finite-difference models
- finite-element models
- boundary-element models
- particle tracking models
  - method-of-characteristics models
  - random walk models, and
- integrated finite-difference models.

The main features of the various numerical models are:

1. The solution is sought for the numerical values of state variables only at specified points in the space and time domains defined for the problem (rather than their continuous variations in these domains).
2. The partial differential equations that represent balances of the considered extensive quantities are replaced by a set of algebraic equations (written in terms of the sought, discrete values of the state variables at the discrete points in space and time).
3. The solution is obtained for a specified set of numerical values of the various model coefficients (rather than as general relationships in terms of these coefficients).
4. Because of the large number of equations that must be solved simultaneously, a computer program is prepared.

In recent years, codes have been developed for almost all classes of problems encountered in the management of ground water. Some codes are very comprehensive and can handle a variety of specific problems as special cases, while others are tailor-made for particular problems. Many of them are available in the public domain, or for a nominal fee. More recently, many codes have been developed or adapted for microcomputers.

Uncertainty

Much uncertainty is associated with the modeling of a given problem. Among them, uncertainties exist in

- the transport mechanisms;
- the various sink/source phenomena for the considered extensive quantity;
- the values of model coefficients, and their spatial (and sometimes temporal) variation;
- initial conditions;
- the location of domain boundaries and the conditions prevailing on them;
- the meaning of measured data employed in model calibration; and
- the ability of the model to cope with a problem in which the solid matrix heterogeneity spans a range of scales,

sometimes orders of magnitude apart.

The degree of uncertainty is increased in most cases by the lack of sufficient data for parameter estimation and model validation. Errors in observed data used for parameter identification also contribute to uncertainty in the estimated values of model parameters.

Various methods for introducing uncertainty into the models and the modeling process have been proposed. For example, one approach is to employ Monte Carlo methods in which the various possibilities are represented in a large number of simulated realizations. Another approach is to construct stochastic models in which the various coefficients are represented as probability distributions rather than deterministic values.

Often the question is raised as to whether, in view of all these uncertainties, which always exist in any real-world problem, models should still be regarded as reliable tools for providing predictions of real-world behavior--*there is no alternative!* However, the kind of answers models should be expected to provide and the very objectives of employing models, should be broadened beyond the simple requirement that they provide the predicted response of the system to the planned excitations. Stochastic models provide probabilistic predictions rather than deterministic ones. Management must then make use of such predictions in the decision-making process. Methodologies for evaluating uncertainties will have to be developed; especially methods for evaluating the worth of data in reducing uncertainty. It then becomes a management decision whether or not to invest more in data acquisition.

In view of the uncertainty involved in modeling, models should be used for additional roles, beyond predicting or estimating the deterministic or probabilistic responses to planned excitations. Such roles include:

- predicting trends and direction of changes;
- providing information on the sensitivity of the system to variations in various parameters, so that more resources can be allocated to reduce their uncertainty;
- deepening our understanding of the system and of the phenomena of interest that take place within it; and
- improving the design of observation networks.

Many researchers are currently engaged in developing methods that incorporate the element of uncertainty in both the forecasting and the inverse models (Freeze et al., 1989; Gelhar, 1986; Yeh, 1986; Neuman et al., 1987, and others).

Model Misuse

As stated above, the most crucial step in ground-water modeling is the development of the conceptual model. If the conceptual model is wrong (i.e., does not represent the relevant flow and contaminant transport phenomena), the rest of the modeling efforts — translating the conceptual model into mathematical and numerical models, and solving for cases of interest — are a waste of time and money. However, mistakes and misuses may occur during any phase of the modeling process (Mercer, 1991).

Following is a list of the more common misuses and mistakes related to modeling. They may be divided into four categories (Mercer and Faust, 1981):

1. Improper conceptualization of the considered problem:
   - improper delineation of the model's domain;
   - wrong selection of model geometry: a 2-D horizontal model, or a 3-D model;
   - improper selection of boundary conditions;
   - wrong assumptions related to homogeneity and isotropy of aquifer material;
   - wrong assumptions related to the significant processes, especially in cases of contaminant transport. These may include the type of sink/source phenomena, chemical and biological transformations, fluid-solid interactions, etc.; and
   - selecting a model that involves coefficients that vary in space, but for which there are insufficient data for model calibration and parameter estimation.
2. Selection of an inappropriate code for solving the model:
   - selecting a code much more powerful/versatile than necessary for the considered problem;
   - selection of a code that has not been verified and tested.
3. Improper model application:
   - selection of improper values for model parameters and other input data;
   - misrepresentation of aquitards in a multi-layer system; mistakes related to the selection of grid size and time steps;
   - making predictions with a model that has been calibrated under different conditions;
   - making mistakes in model calibration (history matching); and
   - improper selection of computational parameters (closure criterion, etc.).
4. Misinterpretation of model results:
   - wrong hydrological interpretation of model results;
   - mass balance is not achieved.

Sources of Information

In selecting a code, its applicability to a given problem and its efficiency in solving the problem are important criteria. In evaluating a code's applicability to a problem and its efficiency, a good description of these characteristics should be accessible. For a large number of ground-water models, such information is available from the International Ground Water Modeling Center (IGWMC, Institute for Ground-Water Research and Education, Colorado School of Mines, Golden, Colorado 80401), which operates a clearinghouse service for information and software pertinent to ground-water modeling. Information databases have been developed to efficiently organize, update and access information on ground-water models for mainframe and microcomputers. The model annotation databases have been developed and maintained over the years with major support from U.S. EPA's Robert S. Kerr Environmental Research Laboratory (RSKERL), Ada, Oklahoma.

The Center for Subsurface Modeling Support (CSMoS) , located at the RSKERL (P.O. Box 1198, Ada, OK 74820), provides ground-water and vadose zone modeling software and services to public agencies and private companies throughout the nation. CSMoS primarily manages and supports ground-water models and databases resulting from research at RSKERL. CSMoS integrates the expertise of individuals in all aspects of the environmental field in an effort to apply models to better understand and resolve subsurface problems. CSMoS is supported internally by RSKERL scientists and engineers, and externally by the IGWMC, National Center for Ground Water Research and numerous ground-water modeling consultants from academia and the private consulting community.

The National Ground Water Information Center (NGWIC, 6375 Riverside Drive, Dublin, Ohio 43017) is an information-gathering and dissemination business that performs customized literature searches on various ground-water-related topics, and locates and retrieves copies of available documents. The center maintains its own on-line databases.

Appendix A: Suggested Format for a Ground-Water Modeling Report

Following is a suggested standardized format for a report that involves modeling and analysis of model results. The emphasis is on the modeling efforts and related activities. It is not an attempt to propose a structure for a project report. The Ground Water Modeling Section (D-18.21.10) of the American Society of Testing and Materials (ASTM) Subcommittee on Ground Water and Vadose Zone Investigations is in the process of developing standards on ground-water modeling. Additionally, specific infor-mation regarding the content of ground-water modeling studies is addressed by Anderson and Woessner (1992, Chapter 9).

Introduction

The introduction may start with a description of the problem that lead to the investigations. The description will include the domain in which the phenomena of interest take place, and what decisions are contemplated in connection with these phenomena. The description should also include information about the geography, topography, geology, hydrology, climate, soils, and other relevant features (of the domain and the considered transport phenomena). Sources of information should be given. The description of the problem should lead to the kind of information that is required by management/decision maker, which the investigations described in the report are supposed to provide.

This section should continue to outline the methodology used for obtaining the required information. In most cases, a model of the problem domain and the transport (i.e., flow and contaminant) phenomena will be the tool for providing management with the required information. On the premise that this section concludes that such a model is needed, the objective of the report is to describe the construction of the model, the model runs, and the results leading to the required information.

Previous Studies

This section should contain a description of earlier relevant studies in the area, whether on the same problem or in connection with other problems. The objective of this section is to examine the data and conclusions in these investigations, as far as they relate to the current study.

The Conceptual Model

Because the previous section concluded that a model is required, the objective of this section is to construct the conceptual model of the problem, including the problem domain and the transport phenomena taking place within it. The content of a conceptual model has been outlined in the text. However, the importance of the conceptual model cannot be overemphasized. It is possible that the existing data will indicate more than one alternative model, if the available data (or lack of it) so dictates.

The Mathematical Model

The conceptual model should be translated into a complete, well-posed mathematical one. At this stage, the various terms that appear in the mathematical model should be analyzed, with the objective of deleting non-dominant effects. Further simplifying assumptions may be added to the original conceptual model at this stage.

If more than one conceptual model has been visualized, a corresponding mathematical model should be presented for each. This section should conclude with a list of coefficients and parameters that appear in the model. The modeler should then indicate for which coefficients values, or at least initial ones, are available (including the actual numerical value and the source of information), and for which coefficients the required information is missing. In addition, the kind of field work or exploration required to obtain that information should be reported. If possible, an estimate should be given for the missing values, their possible range, etc. At this stage, it is important to conduct and report a sensitivity analysis in order to indicate the significance of the missing information, bearing in mind the kind of information that the model is expected to provide.

Selection of Numerical Model and Code

The selected numerical model and the reasons for preferring it over other models (public domain or proprietary) should be presented. Some of the questions that should be answered are: Was the code used as is, or was it modified for the purpose of the project? What were the modifications? If so stated in the contract, the modified code may have to be included in the appendix to the report. The full details of the code (name, version, manual, author, etc.) should be supplied. This section may include a description of the hardware used in running the code, as well as any other software (pre- and post-processors). More information about model selection can be found in Simmons and Cole (1985), Beljin and van der Heijde (1991).

Model Calibration

Every model must be calibrated before it can be used as a tool for predicting the behavior of a considered system. During the calibration phase, the initial estimates of model coefficients may be modified. The sensitivity analysis may be postponed until a numerical model and a code for its solution have been selected.

In this section objectives of the calibration or history matching, the adjusted parameters/coefficients, the criterion of the calibration (e.g., minimizing the difference between observed and predicted water levels), the available data, the model calibration runs, etc., should be described.

The conclusions should be the modified set of parameters and coefficients to be used in the model.

Model Runs

Justification and reasoning for the various runs.

Model Results

This section includes all tables and graphic output. Ranges and uncertainties in model results should be indicated. Results of sensitivity analysis and the significance of various factors should also be discussed.

Conclusions

The information required by the decision maker should be clearly outlined.

Appendices

Tables and graphs, figures, and maps not presented in the body of the report, along with a list of symbols, references, codes, etc., should be included.

Appendix B: Selected Bibliography

Anderson, M.P. 1979. Using Models to Simulate the Movement of Contaminants through Ground Water Flow Systems. Critical Reviews in Environmental Control, v. 9, no. 2, pp. 97-156.

Anderson, M.P. 1984. Movement of Contaminants in Groundwater: Groundwater Transport - Advection and Dispersion. *In* Groundwater Contamination, Studies in Geophysics, National Academy Press, Washington, D.C.

Anderson, M.P. and W.W. Woessner. 1992. Applied Groundwater Modeling. Academic Press, Inc. San Diego, California.

Appel, C.A. and T.E. Reilly. 1988. Selected Reports That Include Computer Programs Produced by the U.S. Geological Survey for Simulation of Ground-Water Flow and Quality. WRI 87-4271. U.S.G.S., Reston, Virginia.

Bear, J. 1972. Dynamics or Fluids in Porous Media. American Elservier, New York, New York.

Bear, J. 1979. Hydraulics of Groundwater. McGraw-Hill, New York.

Bear, J. and A. Verruijt. 1987. Modeling Groundwater Flow and Pollution. Kluwer Academic Publishers, Hingham, Massachusetts.

Bear, J. and Y. Bachmat. 1990. Introduction to Modeling of Transport Phenomena in Porous Media. Kluwer Academic Publishers, Hingham, Massachusetts.

Beck, M.B. 1985. Water Quality Management: A Review of the Development and Application of Mathematical Models. IIASA 11, Springer-Verlag, Berlin, West Germany.

Beljin, M.S. and P.K.M. van der Heijde. 1989. Testing, Verification, and Validation of Two-Dimensional Solute Transport Models. *In* (G. Jousma et al., eds.) Groundwater Contamination: Use of Models in Decision-Making. Kluwer Academic Publishers, Hingham, Massachusetts.

Beljin, M.S. and P.K.M. van der Heijde. 1991. Selection of Groundwater Models for WHPA Delineation. Proc. the AWWA Computer Conference, Houston, Texas.

Boonstra, J. and N.A. De Ridder. 1981. Numerical Modelling of Groundwater Basins, International Institute for Land Reclamation and Improvement, Wageningen, The Netherlands.

Boutwell, S.H., S.M. Brown, B.R. Roberts, and D.F. Atwood. 1985. Modeling Remedial Actions of Uncontrolled Hazardous Waste Sites. EPA 540/2-85/001, U.S. Environmental Protection Agency, Cincinnati, Ohio.

de Marsily, G. 1986. Quantitative Hydrogeology. Academic Press, Inc., Orlando, Florida.

Domenico, P.A. 1972. Concepts and Models in Groundwater Hydrology. McGraw-Hill, New York, New York.

Freeze, R.A., G. DeMarsily, L. Smith, and J. Massmann. 1989. Some Uncertainties About Uncertainty. *In* (B.E. Buxton, ed.) Proceedings of the Conference Geostatistical, Sensitivity, and Uncertainty Methods for Ground-Water Flow and Radionuclide Transport Modeling, San Francisco, California, CONF-870971, Battelle Press, Columbus, Ohio.

Gelhar, L.W., A.L. Gutjahr, and R.L. Naff. 1979. Stochastic Analysis of Macrodispersion in Aquifers. Water Resources Research, v. 15, no. 6, pp. 1387-1397.

Gelhar, L.W. 1984. Stochastic Analysis of Flow in Heterogeneous Porous Media. *In* (J.Bear and M.Y. Corapcioglu, eds.) Fundamentals of Transport Phenomena in Porous Media, Marinus Nijhoff Publishers, Dordrecht, The Netherlands.

Gelhar, L.W. 1986. Stochastic Subsurface Hydrology from Theory to Applications. Water Resources Research, v. 22, no. 9, pp. 135S-145S.

Gorelick, S.M. 1983. A Review of Distributed Parameter Groundwater Management Modeling Methods. Water Resources Research, v. 19, no. 2, pp. 305-319.

Grove, D.B. and K.G. Stollenwerk. 1987. Chemical Reactions Simulated by Ground-Water Quality Models. Water Resources Bulletin, v. 23, no. 4, pp. 601-615.

Herrling, B. and A. Heckele. 1986. Coupling of Finite Element and Optimization Methods for the Management of Groundwater Systems. Advances in Water Resources, v. 9, no. 4, pp. 190-195.

Hunt, B. 1983. Mathematical Analysis of Groundwater Resources. Butterworths Publishers, Stoneham, Massachusetts.

Huyakorn, P.S. and G.F. Pinder. 1983. Computational Methods in Subsurface Flow. Academic Press, New York.

Huyakorn, P.S., B.H. Lester, and C.R. Faust. 1983. Finite Element Techniques for Modeling Ground Water Flow in Fractured Aquifers. Water Resources Research, v. 19, no. 4, pp. 1019-1035.

Istok, J. 1989. Groundwater Modeling by the Finite-Element

Method. AGU Water Resources Monograph 13, American Geophysical Union, Washington, D.C.
Javandel, I., C. Doughty, and C.F. Tsang. 1984. Groundwater Transport: Handbook of Mathematical Models. AGU Water Resources Monograph 10, American Geophysical Union, Washington, D.C.
Keely, J.F. 1987. The Use of Models in Managing Ground-Water Protection Programs. EPA/600/8-87/003.
Kinzelbach, W. 1986. Groundwater Modeling: An Introduction with Sample Programs in BASIC. Elsevier Publication Company, Amsterdam, The Netherlands.
Konikow, L.F. and J.D. Bredehoeft. 1978. Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water. USGS Techniques of Water-Resources Investigations. Book 7, Chap. C2, 90 pp.
Ligget, J.A. and P.L-F. Liu. 1983. The Boundary Integral Equation Method for Porous Media Flow. Allen and Unwin, Inc., Winchester, Massachusetts.
Mercer, J.W. and C.R. Faust. 1981. Ground-Water Modeling. National Water Well Association (NWWA), Worthington, Ohio.
Mercer, J.W., S.D. Thomas, and B. Ross. 1982. Parameters and Variables Appearing in Repository Siting Models. Report NUREG/CR-3066, U.S. Regulatory Commission, Washington, D.C.
Mercer, J.W. 1991. Common Mistakes in Model Applications. Proc. ASCE Symposium on Ground Water, Nashville, Tennessee, July 29 - August 2, 1991.
Moore, J.E. 1979. Contribution of Ground-water Modeling to Planning. Journal of Hydrology. v. 43 (October), pp.121-128.
Narasimhan, T.N. and P.A. Witherspoon. 1976. An Integrated Finite-Difference Method for Analyzing Fluid Flow in Porous Media. Water Resources Research v. 12, no. 1, pp. 57-64.
Narasimhan, T.N. 1982. Numerical Modeling in Hydrogeology. *In* T.N. Narasimhan (ed.), Recent Trends in Hydrogeology, pp. 273-296, Special Paper 189 Geological Society of America, Boulder, Colorado.
National Research Council (NRC). 1990. Ground Water Models: Scientific and Regulatory Application. National Research Council, Water Science and Technology Board, Washington, D.C.
Neuman, S.P., C.L. Winter, and C.M. Newman. 1987. Stochastic Theory of Field-Scale Fickian Dispersion in Anisotropic Porous Media. Water Resources Research, v. 23, no. 3, pp. 453-466.
Pickens, J.F. and G.E. Grisak. 1981. Modeling of Scale-Dependent Dispersion in Hydrologic Systems. Water Resources Research, v. 17, no. 6, pp. 1701-1711.
Pinder, G.F. and J.D. Bredehoeft. 1968. Application of the Digital Computer for Aquifer Evaluation. Water Resources Research. v. 4, no. 5, pp. 1069-1093.
Pinder, G.F. and W.G. Gray. 1977. Finite Element Simulation in Surface and Subsurface Hydrology. Academic Press, New York, 295 pp.
Pinder, G.F. and L. Abriola. 1986. On the Simulation of Nonaqueous Phase Organic Compounds in the Subsurface. Water Resources Research, v. 22, no. 9, pp. 1092-1192.
Prickett, T.A. 1975. Modeling Techniques for Groundwater Evaluation. *In* Ven Te Chow (ed.), Advances in Hydroscience, Vol. 10.
Prickett, T.A. and C.G. Lonnquist. 1982. A Random-Walk Solute Transport Model for Selected Groundwater Quality Evaluations. Bull. No. 65, Illinois State Water Survey, Urbana, 105 pp.
Remson, I., G.M. Hornberger, and F.J. Molz. 1971. Numerical Methods in Subsurface Hydrology. John Wiley and Sons, New York, New York.
Rushton, K.R. and S.C. Redshaw. 1979. Seepage and Groundwater Flow: Numerical Analysis by Analog and Digital Methods. John Wiley and Sons, Chichester, U.K.
Schmelling, S.G. and R.R. Ross. 1989. Contaminant Transport in Fractured Media: Models for Decision Makers. USEPA Superfund Ground Water Issue Paper. EPA/540/4-89/004.
Simmons, C.S. and C.R. Cole. 1985. Guidelines for Selecting Codes for Ground-Water Transport Modeling of Low-Level Waste Burial Sites. PNL-4980, Volume I and II, Battelle Pacific Northwest Labs, Richland, Washington.
Strack, O.D.L. 1989. Groundwater Mechanics. Prentice Hall, Englewood Cliffs, New Jersey.
Trescott, P.C., G.F. Pinder, and S.P. Larson. 1976. Finite-Difference Model for Aquifer Simulation in Two-Dimensions with Results of Numerical Experiments. U.S.G.S. Techniques of Water Resources Investigation, Book 7, Chap. C1, 116 pp.
U.S. Office of Technology Assessment. 1982. Use of Models for Water Resources Management, Planning, and Policy. U.S. OTA for Congress of the United States, U.S. Government Printing Office, Washington, D.C.
van der Heijde, P.K.M. et al. 1985. Groundwater Management: The Use of Numerical Models. 2nd edition, AGU Water Resources Monograph no. 5, Washington, D.C.
van der Heijde, P.K.M. and M.S. Beljin. 1988. Model Assessment for Delineating Wellhead Protection Areas. EPA/440/6-88-002. Office of Ground Water Protection, U.S. Environmental Protection Agency, Washington, D.C.
van der Heijde, P.K.M., A.I. El-Kadi, and S.A. Williams. 1989. Groundwater Modeling: An Overview and Status Report. EPA/600/2-89/028. R.S. Kerr Environmental Research Lab, U.S. Environmental Protection Agency, Ada, Oklahoma.
van Genuchten, M.Th. and W.J. Alves. 1982. Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation. U.S. Dept. of Agriculture, Tech. Bull. No. 1661.
Walton, W. 1985. Practical Aspects of Ground Water Modeling. Lewis Publishers, Chelsea, Michigan.
Walton, W. 1989. Analytical Ground Water Modeling. Lewis Publishers, Chelsea, Michigan.
Wang, H.F. and M.P. Anderson. 1982. Introduction to Groundwater Modeling. W.H. Freeman and Co., San Francisco, California.
Yeh, W. W-G. 1986. Review of Parameter Identification Procedures in Groundwater Hydrology: The Inverse Problem. Water Resources Research, v. 22, no. 2, pp. 95-108.