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CHAPTER 10

NUMERICAL MODELING OF CONTAMINANT TRANSPORT

10.1 INTRODUCTION

A ground water model is a tool designed to represent a simplified version of a real field site. It is an attempt to take our understanding of the physical, chemical, and biological processes and translate them into mathematical terms. The resulting model is only as good as the conceptual understanding of the processes. The goal of modeling is to predict the value of an unknown variable such as head in an aquifer system or the concentration distribution of a given chemical in the aquifer in time and space. Models can be used as:

1. Predictive Tools. These are site specific applications of models with the objective of determining future conditions or the impact of a proposed action on existing conditions in the subsurface.

2. Interpretive or Research Tools. These models are usually used for studying system dynamics and understanding processes.
3. Generic or Screening Tools. These models generally incorporate uncertainty in aquifer parameters and are used in a regulatory mode for the purpose of developing management standards and guidelines.

In developing a ground water flow or solute transport model, the first step is to develop a **conceptual model** consisting of a description of the physical, chemical and biological processes which are thought to be governing the behavior of the system being analyzed (Istok, 1989). The next step is to translate the conceptual model into mathematical terms or a **mathematical model**, that is, a set of partial differential equations and an associated set of auxiliary boundary conditions. Finally, solutions of the equations subject to the auxiliary conditions can be obtained using analytical or numerical methods.

If analytical methods are used, the solution is called an **analytical model**. Analytical solutions are usually possible only for simple geometries, homogeneous aquifers, and simple boundary conditions. If numerical methods are used, the solution to the collection of partial differential equations and auxiliary conditions is referred to as a **numerical model.** A computer program that implements the numerical model is referred to as a **computer code** or **computer model**. Computer models are essential for analyzing subsurface flow and contamination problems because they are designed to incorporate the spatial variability within the aquifer, as well as spatial and temporal trends in hydrologic parameters that an analytical model cannot incorporate.

Much discussion has been presented over the past decade regarding the usefulness and drawbacks of modeling. The main complaint of models is that they require great quantities of data and are therefore too expensive to assemble and run. Furthermore, models can never be proven to be correct. On the other hand, some argue that models are essential for performing complex analyses and for making informed decisions. Models allow more effective use of the available data; the implications of proposed courses of action at the field scale can be analyzed and evaluated with them.

Both arguments are well justified. The prospective modeler, however, needs to keep in mind that a good modeling methodology will increase confidence in modeling results. In addition, establishing the purpose of the modeling effort at the outset and establishing realistic expectations will provide for a much more effective utilization of modeling. Prior to initiating the modeling process, the following questions need to be addressed:

1. What is the problem that is being solved or answered through modeling?
2. Is modeling the most appropriate method for establishing the answer to the problem at hand?
3. What level of sophistication in modeling would be required to answer the question?
4. What level of confidence can be associated with the available field data and the anticipated results from the modeling effort?

The responses to these questions will allow the prospective modeler to determine the magnitude of the modeling effort, that is, whether the model is one-, two-, or three-dimensional, analytical or numerical, and whether a steady-state or transient analysis is necessary. Answering question #4 allows the modeler to anticipate the benefits to be gained from the modeling effort and to weigh those benefits against the costs that would be incurred for the modeling study. Finally, keep in mind that modeling is only one component in a hydrogeologic assessment and not an end in itself. The proposed modeling effort should be integrated within the framework for action at a given field site.

The field of ground water flow and transport modeling has grown tremendously over the past fifteen years. This is mostly due to the need for quantitative estimates of flow and mass transport in the subsurface. Many articles and books have been written about the science of modeling in ground water. The reader is referred to Mercer and Faust (1986), Wang and Anderson (1982), Huyakorn and Pinder (1983), Hunt (1983), Javandel et al. (1984), Bear and Verruijt (1987), Istok (1989), National Research Council (1990), and Anderson and Woessner (1992) as a starting point. Anderson and Woessner (1992) propose a modeling protocol that can be summarized as follows:

1. Establish the purpose of the model.
2. Develop a conceptual model of the system.
3. Select the governing equation and a computer code. Both the governing equation and code should be verified. Verification of the governing equation demonstrates that it describes the physical, chemical, and biological processes occurring. Code verification can be accomplished by comparing the model results to an analytical solution of a known problem.
4. Design the model. This step includes selection of a grid design, time parameters, initial and boundary conditions, and developing estimates of model parameters.
5. Calibrate the designed model. Calibration refers to the process of determining a set of model input parameters that approximates field measured heads, flows and/or concentrations. The purpose of calibration is to establish that the model can reproduce field-measured values of the unknown variable. It is noted that calibration is quite subjective and in many cases does not yield a unique set of parameters that reproduce field conditions. This topic will be discussed in more detail in Section 10.9.
6. Determine the effects of uncertainty on model results. This is sometimes referred to as a sensitivity analysis. The model parameters are varied individually within a range of possible values, and the effect on model results is evaluated.
7. Verify designed and calibrated model. This step involves testing the model's ability to reproduce another set of field measurements using the model parameters that were developed in the calibration process.

8. Predict results based on calibrated model.
9. Determine the effects of uncertainty on model predictions.
10. Present modeling design and results.
11. Post audit and redesign model as necessary. As more data is collected beyond model development, it is possible to compare the model predictions against the new field data. This may lead to further modifications and refinements of the site model.

Steps 1 through 4 of Anderson and Woessner's protocol are discussed in this section. The remaining steps are discussed in Section 10.9 within the context of applying models to field sites.

10.1.1 Purpose of Model

It is essential to identify clearly the purpose of the modeling effort at the outset in order to maximize the benefits from the analysis. Stating the purpose of modeling also helps focus the study, determine expectations, and limit the unnecessary expenditure of resources. Typical objectives for modeling studies include:

1. Testing a hypothesis, or improving knowledge of a given aquifer system
2. Understanding physical, chemical or biological processes
3. Designing remediation systems
4. Predicting future conditions or the impact of a proposed stress on a ground water system
5. Resource management

10.1.2 Conceptual Models

A key step in the modeling process is to formulate a conceptual model of the system being modeled. A conceptual model is a pictorial representation of the ground water flow and transport system, frequently in the form of a block diagram or a cross section (Anderson and Woessner, 1992). The nature of the conceptual model will determine the dimensions of the numerical model and the design of the grid.

The purpose of building a conceptual model is to simplify the field problem and make it more amenable to modeling. For example, consider the geologic framework shown in Figure 10.1. A complete reconstruction of this system in a ground water flow model is not feasible; however, a conceptual model of the system can be constructed by identifying the pertinent hydrologic features of the geologic framework as shown in Figure 10.1.

Formulating a conceptual model for flow and/or transport includes one or more of the following steps depending on the nature of the problem being simulated:

1. Define hydrogeologic features of interest, (e.g., the aquifers to be modeled). The conceptual model may combine several geologic formations into a single unit or may subdivide a single formation into aquifers and confining units.
2. Define the flow system and sources and sinks of water in the system. Sources or inflows may include recharge from infiltration, recharge from surface water bodies, or artificial recharge of ground water. Sinks or outflows may include springflow, baseflow to streams, evapotranspiration, and pumping. Defining the flow system involves determining the direction of ground water flow and the hydrologic interaction between the different modeled units.
3. Define the transport system and sources and sinks of chemicals in the system. The conceptual model has to include a representation of the time-variant chemical source concentration, mass or volume of spill, and the chemical and biological processes affecting those chemicals.

Recent advances in software development have resulted in the ability to build a conceptual model and manage site data within a model pre- and post-processor or a Geographical Information System (GIS), which can interact with the pre-processor. This type of software is discussed in Section 10.8.

10.1.3 Equations of Flow and Transport

As mentioned earlier, one of the steps in the modeling protocol is to determine the governing equation to be solved. This is extremely important, especially when the modeler is applying a model that has been acquired from a commercial source. A review of three of the classes of models based on the processes being modeled and the associated governing equations is presented next. The reader is referred to Chapters 9 and 11 for the immiscible/multiphase flow and transport equations.

Saturated Ground Water Flow in Three Dimensions:

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)=S_s\frac{\partial h}{\partial t}+W^* \tag{10.1}$$

where h is head, K_x, K_y, K_z, denote hydraulic conductivity in the x-, y-, and z- directions, respectively, S_s is specific storage, t is time, and W^* is a general source/sink term.

Unsaturated Ground Water Flow Equation in Three Dimensions:

$$\frac{\partial}{\partial x}\left(K_x(\psi)\frac{\partial \psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y(\psi)\frac{\partial \psi}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z(\psi)\left(\frac{\partial \psi}{\partial z}\right)\right)=C(\psi)\frac{\partial \psi}{\partial t}\pm Q \tag{10.2}$$

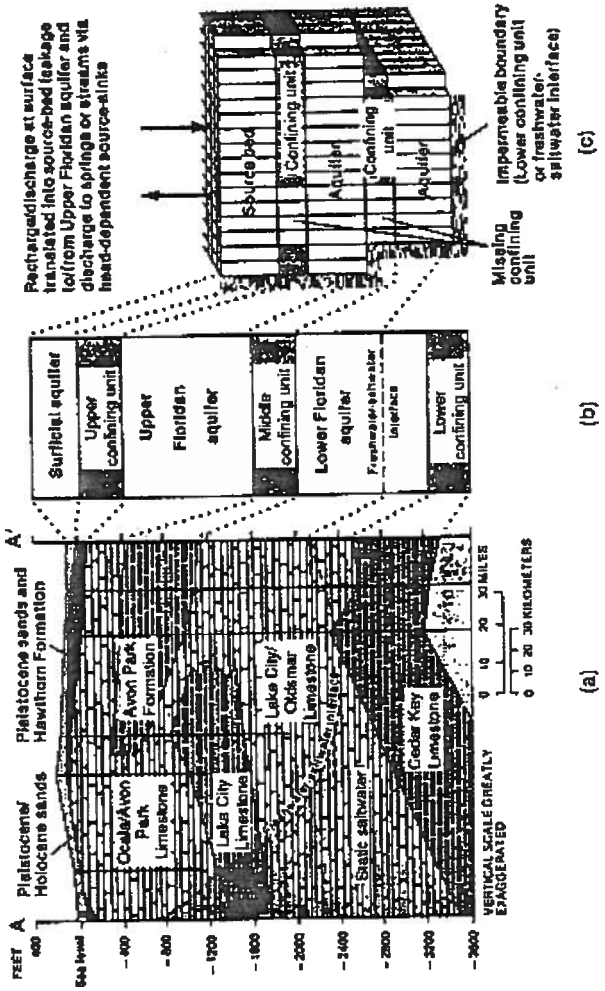

Figure 10.1 Developing a hydrogeologic conceptual model. (a) Geologic units in hydrogeologic framework. (b) Hydrogeological units in conceptual model. c) Equivalent units in digital ground water flow model. Source: Anderson and Woessner, 1992.

where ψ is pressure head; $K_x(\psi)$, $K_y(\psi)$, $K_z(\psi)$, are the components of the unsaturated hydraulic conductivity in the x-, y-, and z- directions, respectively; $C(\psi)$ is the specific moisture capacity, and Q is a source or sink of volumetric fluid flow per unit volume.

Solute Transport in the Saturated Zone in Three Dimensions

$$D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}+D_z\frac{\partial^2 C}{\partial z^2}-\frac{\partial(CV_x)}{\partial x}-\frac{\partial(CV_y)}{\partial y}-\frac{\partial(CV_z)}{\partial z}\pm\sum_k R_k=\frac{\partial C}{\partial t} \qquad (10.3)$$

where C is the concentration of the chemical; V is the seepage velocity; D_x, D_y, and D_z are the dispersion coefficients in the x, y, and z directions, respectively; t is time; and R_k is the rate of addition or removal of solute due to chemical and biological reactions.

10.1.4 Discretization

In numerical models, the physical layout of the area in question is replaced with a discretized model domain referred to as a grid and consisting of cells, blocks, or elements depending on whether finite difference or finite element methods are used. Some of the key issues in setting up numerical models have to do with the design of the grid system: How large of a grid to use? How many cells or elements within the grid would be necessary? What impact, if any, does grid discretization have, on model results?

Generally, the grid should be drawn on an overlay of a map of the area to be modeled. It is preferable to align the horizontal plane of the grid such that the x and y axes are collinear with K_x and K_y, respectively. The vertical axis of the model, when present, should be aligned with K_z (Anderson and Woessner, 1992). Selecting the size of the cells/elements to be used is a critical step in grid design that depends on many factors such as: spatial variability in model parameters, physical boundaries of system, type of model being used (finite difference or finite element), computer model limitations, data handling limitations, runtime, and associated computer costs. Spatial discretization may affect model results. While detailed discussion of this issue is beyond the scope of this chapter, the prospective modeler is encouraged to evaluate discretization effects on model results.

Discretization decisions also need to be made for the time parameter. The majority of numerical models calculate results at time t by subdividing the total time into time steps, Δt. Generally, smaller time steps are preferable, but the computational time and cost involved in the modeling process increases as the time step is decreased. Time steps may be influenced by the requirements of the model. Some models suffer from **numerical instabilities,** which cause unrealistic oscillating solutions if a sufficiently small time step is not used. It is a good modeling practice to test the sensitivity of the model results to the size of the time step. Many transport models calculate the maximum time step size based on model conditions, such as grid size and flow velocity. This enables the transport model to eliminate some numerical instability; however, flow models cannot use this method, and must be carefully checked by the user.

10.1.5 Dimensionality

Another issue closely linked to discretization is that of the dimensionality of the problem: is a 1-D model sufficient to achieve the purposes of modeling or is it necessary to develop a 2-D or 3-D model? Would an analytical solution provide the required answer or is it necessary to utilize a numerical model? Is a steady-state assumption adequate or does the problem necessitate a transient analysis?

A good rule of thumb to use when deciding the dimensionality of the model is to avoid complexity if at all possible. For example, air pollution modeling might require a three-dimensional analysis of pollutant dispersion and diffusion. Ground water contamination at a field site where the data has been collected using conventional monitoring wells, however, can be simulated only as a 2-D problem because there is not a 3-D definition of the plume of contamination.

10.1.6 Boundary and Initial Conditions

The governing equation alone is not sufficient to describe a specific physical system. This is because a general solution of an n^{th} order differential equation will involve n independent arbitrary constants or functions. In order to define uniquely a given physical problem, the values of the constants or forms of the functions must be specified. Initial and boundary conditions can be used to provide this required additional information. Generally, boundary conditions specify the value of the dependent variable, or the value of the first derivative of the dependent variable, along the boundaries of the system being modeled.

Correct selection of boundary conditions is a critical step in model design. In steady-state simulations, for example, the boundaries largely determine the flow pattern. Boundary conditions affect transient solutions when the effects of the transient stress reach the boundary. In this case, the boundaries must be selected such that the simulated effect is realistic.

Boundary conditions are typically derived from physical and/or hydraulic boundaries of ground water flow systems, for example, the presence of an impermeable body of rock or a river in connection with the ground water aquifer. Hydrogeologic boundaries are represented by three types of mathematical formulations: specified head, specified flux, and head dependent flux boundaries.

Specified head. (Dirichlet conditions). A specified head boundary is simulated by setting the head at the relevant locations equal to known values:

$$H(x, y, z) = H_0 \tag{10.4}$$

where $H(x, y, z)$ is the head at a point with coordinates (x, y, z) and H_0 is a specified head value. It is important to recognize that a specified head boundary represents an inexhaustible supply of water.

Specified flux boundaries. (Neumann conditions). Specified flux boundaries are defined by giving the derivative of the head across the boundary:

$$q_x = \frac{\partial H}{\partial x} = \text{Constant} \tag{10.5}$$

This type of boundary is used to describe fluxes to surface water bodies, springflow and seepage to and from bedrock underlying the system. A special type of specified flux boundaries is a no-flow boundary which is set by specifying flux to be zero. A no-flow boundary may represent impermeable bedrock, an impermeable fault zone, a ground water divide or a streamline.

Head-dependent flux boundaries. (Cauchy or mixed conditions). For this type of boundary, the flux across the boundary is calculated given a boundary head value:

$$\frac{\partial H}{\partial x} + aH = C \tag{10.6}$$

where a and C are constants. Leakage to or from a river, for instance, can be simulated using this type of boundary condition.

In some instances, it may not be possible to use physical boundaries and regional ground water divides. Other hydraulic boundaries can be defined from information on the configuration of the flow system. However, care must be taken when establishing such boundaries to ensure that the model boundaries will not cause the solution to differ significantly from the response that would occur in the field. For example, hydraulic boundaries may be defined from a water table map of the area to be modeled. The model grid is superimposed on the water table contour map, and specified head boundary conditions can be interpolated. It is important to verify, however, that these boundary conditions will not be impacted by stresses imposed on the model, such as pumping from a location near the boundary.

The above mentioned boundary conditions used to represent flow may also be used as sources of chemicals into a ground water aquifer. For example, a specified head boundary may be used to represent a contaminant source releasing chemicals into the aquifer at a specified concentration. Similarly, a flux boundary can be used to simulate the flux of contaminants across the boundary. More typically, however, injection wells are used to represent sources of contamination as discussed in the following paragraphs.

10.1.7 Sources and Sinks

Water as well as chemicals may enter the grid in one of two ways — through the boundaries, as determined by the boundary conditions, or through sources and sinks within the interior of the grid. Even though the same model options may be used to represent boundary sources and sinks as to represent internal sources and sinks, the reader should remember that internal sources and sinks are not boundary conditions. For example, specified head cells are used to represent specified head boundary conditions, but specified head nodes may be placed within the grid to represent lakes and rivers or some other type of source.

An injection or pumping well is a point source or sink and is represented in a ground water model by specifying an injection or pumping rate at a designated node or cell. In a 2-D model, an assumption of a fully penetrating well over the aquifer thickness is made. The prospective modeler is cautioned when modeling wells with models that allow only a uniform grid (i.e., all cells have the same size), and when the cell size in the model greatly exceeds the actual diameter of the well. The head calculated by the model is not an accurate approximation of the head measured in the well, but rather the head value predicted by the model is closer to an average of the heads measured as one moves outward from the well toward the edge of the cell.

10.1.8 Source and Types of Errors: Accuracy of Numerical Models

One of the key components in computer modeling of ground water flow and contaminant transport that is often neglected is an assessment of the error introduced due to the selected modeling methodology. There are two types of error resulting from a modeling study that need to be clearly distinguished:

1. Computational errors. These errors occur because of the numerical approximation procedures that are used to solve the governing equations. Computational errors are usually estimated by applying the continuity equation or the principle of conservation of mass (input – output = accumulation).
2. Calibration errors. These errors occur due to model assumptions and limitations in parameter estimation. Calibration errors can be quantified by comparing the model's predicted values to observed values of the unknown variable (see Section 10.9).

10.1.9 Limitations of Models

Mathematical models have several limitations, which can be conceptual or application-related. Conceptual limitations are those that relate to representation of the actual process or system with a mathematical model. For example, analytical models are limited by the simplifying assumptions that are required to develop the solution. The analytical models that are available are limited to certain idealized conditions and may not be applicable to a field problem with complex boundary conditions. Another limitation of analytical models is that spatial or temporal variation of system properties such as permeability and dispersivity cannot be handled.

Application-related limitations have to do with the solution procedure that is utilized in the model development or with the amount of effort required to implement the solution. For example, the approximation of a differential equation by a numerical solution introduces two types of computational errors: numerical and residual. The numerical errors are due to

the solution method used in solving the differential equations. The residual errors are a result of approximating the differential equation with a series of mathematical expressions.

Numerical models are also limited by their complexity so that the user needs a certain level of knowledge to be able to apply those models. Achievement of the required familiarity level is time consuming and could be prohibitive when funding is limited or when dealing with a time constraint. Preparation of input data for numerical models often takes a long time, even with the recently developed pre-processors discussed in Section 10.8. A relatively fast computer is necessary when using a numerical model, especially for large, complex problems.

10.2 NUMERICAL METHODS

Numerical or computerized solutions of the flow and/or transport equation in two dimensions are the most plentiful and commonly used techniques. These solutions are generally more flexible than analytical solutions because the user can approximate complex geometries and combinations of recharge and withdrawal wells by judicious arrangement of grid cells. The general method of solution is to break up the flow field into small cells, approximate the governing partial differential equations by differences between the values of parameters over the network of time t, then predict new values for time $t + \Delta t$. This continues forward in time in small increments Δt.

The most common mathematical formulations for approximating the partial differential equations of flow and solute transport include:

- Finite difference methods
- Finite element methods
- Method of characteristics
- Collocation methods
- Boundary element methods

Before defining these methods, it is necessary to define the different types of Partial Differential Equations (PDEs). All PDEs of the form $L(u) = f$ can be classified as **elliptic, parabolic, or hyperbolic.** The PDE can be written as:

$$a\frac{\partial^2 u}{\partial x^2} + 2b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} = F\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) \tag{10.7}$$

where a, b, and c are functions of x and y only and the equation is classified as linear if F is linear. The PDE is referred to as:

- Hyperbolic, if $b^2 - ac > 0$
- Parabolic, if $b^2 - ac = 0$
- Elliptic, if $b^2 - ac < 0$

The finite difference method is the most popular method for simulating problems of ground water flow and transport. Finite difference methods are conceptually straightforward and easily understood. Moreover, much research has been done on developing a variety of algorithms for solving finite difference equations. The earlier finite-difference methods operate by dividing space into rectilinear cells along the coordinate axes. Homogeneous values within each cell are represented by values at a single node. Partial differentials can then be approximated by differences and the resulting set of equations solved by iteration (Mercer and Faust, 1986; Carnahan et al., 1969; Prickett, 1975). Approximating the differentials by a difference requires neglecting remaining terms, which results in **truncation** error.

Finite-difference models have been developed for a variety of field situations including saturated and unsaturated flow, and for transient and constant pollutant sources. The primary disadvantage of these methods is that the truncation error in approximating the partial differential equations be significant (Anderson, 1979). More details about the finite difference method are included in Section 10.3, and the reader is referred to Peaceman and Rachford (1955), Forsythe and Wasow (1960), Aziz and Settari (1979), Crichlow (1977), Peaceman (1977), Remson et al. (1965), Freeze and Witherspoon (1966), Bittinger et al. (1967), Pinder and Bredehoeft (1968), Cooley (1971), Freeze (1971), Brutsaert (1973), Green et al. (1970), Peaceman and Rachford (1962), Shamir and Harleman (1967), Oster et al. (1970), Tanji et al. (1967), and Zheng and Bennett, (1995) for additional information.

The finite element method also operates by breaking the flow field into elements, but in this case the elements may vary in size and shape. In the case of a triangular element, the geometry would be described by the three corner nodes where heads and concentrations are computed. The head or concentration within an element can vary in proportion to the distance to these nodes. Sometimes complex interpolating schemes are used to predict parameter values accurately within an element and thereby reduce the truncation errors common in finite difference procedures. Some numerical dispersion may still occur but is usually much less significant. The use of variable size and shape elements also allows greater flexibility in the analysis of moving boundary problems, such as those related to a moving water table or when contaminant and flow transport must be analyzed as a coupled problem.

A disadvantage of the finite element method is the need for formal mathematical training to understand the procedures properly. Finite element methods generally have higher computing costs (Pinder and Gray, 1977; Pinder, 1973; Wang and Anderson, 1982). More details on the finite element method are presented in Section 10.4, and the reader is additionally referred to Bathe and Wilson (1976), Chung (1979), Clough (1960), Cook (1974), Finlayson (1972), Huebner (1975), Hinton and Owen (1979), Norrie and De Vries (1978), Segerlind (1976), Zienkiewicz (1977), Gallagher (1975), and Zheng and Bennett (1995).

The method of characteristics (MOC) is a variant of the finite difference method and is particularly suitable for solving hyperbolic equations. The method of characteristics was developed to simulate advection-dominated transport by Garder et al. (1964). In ground water hydrology, Pinder and Cooper (1970) and Reddell and Sunada (1970) used the method to solve the density-dependent transport equations. Later, MOC was used widely to simulate the movement of contaminants in the subsurface (Bredehoeft and Pinder, 1973). The method of characteristics is most useful where solute transport is dominated by advective transport. The most common procedure is to track idealized particles through the flow field. In step one, a particle and an associated mass of contaminant are translated a certain distance according to the flow velocity. The second step adds the effects of longitudinal and transverse dispersion. This procedure is computationally efficient and minimizes numerical dispersion problems (Konikow and Bredehoeft, 1978). The method of characteristics is discussed in more detail in Section 10.5.

The collocation method provides the advantage of the finite element method with additional attractive features. Collocation methods do not require integration procedures in the formulation of the approximating equations. Moreover, the resulting matrix equation exhibits a coefficient structure that may be amenable to efficient solution using modern methods in matrix algebra (Huyakorn and Pinder, 1983). The collocation method will not be discussed in detail in this book; however, the reader is referred to Finlayson (1972), Chang and Finlayson (1977), Houstis et al. (1979), Douglas and Dupont (1974), Sincovec (1977), Allen and Pinder (1983), Bangia et al. (1978), Pinder et al. (1978), Frind and Pinder (1979), Lapidus and Pinder (1982), and Celia and Pinder (1980).

The boundary element method, a variant of the finite element method, is especially useful in the solution of elliptic equations for which Green's functions exist. The boundary element method reduces a 2-D or 3-D problem to one defined in one or two dimensions, respectively. The boundary element method is a relative newcomer in applied numerical analysis and not very popular yet in subsurface hydrology. The boundary element method will not be discussed in this book, but the interested reader is referred to Jawson and Ponter (1963), Liggett (1977), Brebbia and Walker (1980), Lapidus and Pinder (1982), Liggett and Liu (1983), Benarjee et al. (1981), Rizzo and Shippy (1970), Dubois and Buysee (1980), Jawson and Symm (1977), Lennon et al. (1979), and Liggett and Liu (1979).

10.2.1 Fundamental Concepts

The following summary is not intended to be a thorough discussion of numerical methods. It is included to familiarize the reader with some of the more common terminology used in numerical modeling. For detailed discussions on numerical methods, the reader is referred to Kelly (1967), Carnahan et al. (1969), Celia and Gray (1992), and Mathews (1992).

Iteration means that a process is repeated until an answer is achieved. Iterative techniques can be used to find roots of equations, solutions of linear and nonlinear systems of equations and solutions of differential equations. Iteration methods require that an initial guess be made and that a rule or function for computing successive terms exists.

Convergence is characterized by the question, "Does the numerical solution approach the true solution as a chosen numerical procedure is applied?" The convergence prob-

lem may arise from using an iterative technique or a numerical technique that involves truncation of an infinite series.

A **stable** numerical procedure is one where as the solution marches forward in time, the errors are not amplified such that the solution becomes invalid.

Curve fitting techniques attempt to fit a given set of data with a mathematical expression or function. For example, one of the most common curve fitting methods is a **least squares fit,** where the function $f(x)$ is approximated using:

$$f(x) \approx \sum_{k=0}^{n} a_k \phi_k(x) \equiv y(x) \tag{10.8}$$

where $\phi_0(x)$,..., $\phi_n(x)$ are $n+1$ appropriately chosen functions. The exact values of $f(x)$ are known over a certain domain, which consists of a discrete set of points x_0, x_1, ..., x_n or of a continuous interval (a, b). The least squares approximation is defined to be that for which the a_k's are determined so that the sum of $w(x)r^2(x)$ the domain is as small as possible, where $w(x)$ is a nonnegative weighting function and $r(x) = f(x) - y(x)$.

Newton-Raphson Iteration involves finding a root of $f(x) = 0$ given one initial approximation p_0 and using the iteration

$$p_k = p_{k-1} - \frac{f(p_{k-1})}{f'(p_{k-1})} \qquad \text{for } k = 1, 2,... \tag{10.9}$$

Secant Method is applied to finding a root of $f(x) = 0$ given two initial approximations p_0 and p_1 and using the iteration

$$p_{k+1} = p_k - \frac{f(p_k)[p_k - p_{k-1}]}{f(p_k) - f(p_{k-1})} \qquad \text{for } k = 1, 2,... \tag{10.10}$$

Gaussian Elimination and Back-Substitution refers to the simplest method of solving a set of equations of the form:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n &= b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \cdots + a_{3n}x_n &= b_3 \\ a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n &= b_n \end{aligned} \tag{10.11}$$

Gaussian elimination consists of dividing the first equation by a_{11} and using the result to eliminate x_1 from all succeeding equations. Next, the modified second equation is used to eliminate x_2 from the succeeding equations, and so on. After this elimination has been effected n times, the resultant set of equations is solved by backward substitution.

10.2.2 The Numerical Solution of Partial Differential Equations

The purpose of this example is to present an introductory account of the numerical methods by which approximate solutions to partial differential equations can be obtained. The fundamental idea on which the numerical solution of partial differential equations is based is this: each of the partial derivatives that appears in the equation is replaced by a finite-difference approximation. When these differences are evaluated at each of the mesh points, the result is a set of simultaneous equations that can be solved either directly or by various iterative procedures.

Specifically, in a plane grid, if the coordinates of the mesh points (named neutrally for the moment) are $p_i = p_0 + ih$ and $q_j = q_0 + jk$, then from the usual difference quotient approximation to the first derivative, we have

$$\left.\frac{\partial u}{\partial p}\right|_{p_i,q_j} = \frac{u_{p_{i+1},q_j} - u_{p_i,q_j}}{h} = \frac{u_{i+1,j} - u_{i,j}}{h} \tag{10.12}$$

Similarly

$$\left.\frac{\partial u}{\partial q}\right|_{p_i,q_j} = \frac{u_{i,j+1} - u_{i,j}}{k} \tag{10.13}$$

Furthermore, for the case of a second derivative, we obtain

$$\left.\frac{\partial^2 u}{\partial p^2}\right|_{p_i,q_j} = \frac{u_{p_{i+1},q_j} - 2u_{p_i,q_j} + u_{p_{i-1},q_j}}{h^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \tag{10.14}$$

Similarly

$$\left.\frac{\partial^2 u}{\partial q^2}\right|_{p_i,q_j} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} \tag{10.15}$$

Elliptic Equations (Laplace's Equation In Two Dimensions). Using Eqs. (10.14) and (10.15) to approximate each of the partial derivatives in the 2-D form of Laplace's equation, namely

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{10.16}$$

We obtain, as a difference equation approximating the actual equation

$$\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2}+\frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{k^2}=0 \tag{10.17}$$

or, making the natural and convenient assumption that $h = k$ and solving for $u_{i,j}$

$$u_{i,j}=\frac{u_{i+1,j}+u_{i,j+1}+u_{i-1,j}+u_{i,j-1}}{4} \tag{10.18}$$

This asserts that the value of u at any mesh point is equal to the average of the values of u at the four adjacent mesh points.

If Eq. (10.18) is evaluated at each of the mesh points, which are not boundary points, where the value of the solution u is initially given, the result is a system of simultaneous linear equations in the unknown functional values $u_{i,j}$. The number of equations is, of course, just equal to the number of mesh points at which the value of u is to be calculated; and (at least for rectangular regions) it can be shown that this system of equations always has a unique nontrivial solution.

Example 10.1 STEADY STATE HEAD IN A SQUARE REGION

To illustrate the formulation and solution of such a system, let us attempt to approximate the steady-state head distribution $u(x,y)$ in the square region shown in Figure 10.2, using the grid obtained by dividing each edge into four equal parts. The unknowns in this problem are the heads at the nine points of the grid which are not boundary points.

Solution. At the outset, we note that from symmetry $u_{11} = u_{31}$, $u_{12} = u_{32}$, and $u_{13} = u_{33}$, so that our problem actually involves only six equations in the six unknowns u_{11}, u_{12}, u_{13}, u_{21}, u_{22}, and u_{23}. Applying Eq. (10.18) at each of the six mesh points P_{11}, P_{12}, P_{13}, P_{21}, P_{22}, P_{23} and taking into account the symmetries we have just noted and the known values of u on the boundary, we have at P_{11}

$$4u_{11}-u_{01}-u_{10}-u_{21}-u_{12}=0$$

or noting that by hypothesis $u_{01} = u_{10} = 0$

$$4u_{11}-u_{21}-u_{12}=0 \tag{10.19}$$

Similarly, at P_{12}, P_{13}, P_{21}, P_{22}, P_{23} we have, respectively

$$4u_{12}-u_{11}-u_{22}-u_{13}=0 \tag{10.20}$$

$$4u_{13}-u_{12}-u_{23}=3/16 \tag{10.21}$$

$$4u_{21}-2u_{11}-u_{22}=0 \tag{10.22}$$

$$4u_{22}-u_{21}-2u_{12}-u_{23}=0 \tag{10.23}$$

$$4u_{23}-u_{22}-2u_{13}=1/4 \tag{10.24}$$

Using Eqs. (10.19), (10.20), and (10.21) to eliminate u_{21}, u_{22}, and u_{23} from Eqs. (10.22), (10.23), and (10.24), we obtain the system

$$15u_{11}-8u_{12}+u_{13}=0$$

$$-8u_{11}+16u_{12}-8u_{13}=-\frac{3}{16}$$

$$15u_{13}-8u_{12}+u_{11}=1$$

Yielding $u_{11} = 0.0154$, $u_{12} = 0.0396$, $u_{13} = 0.0872$.

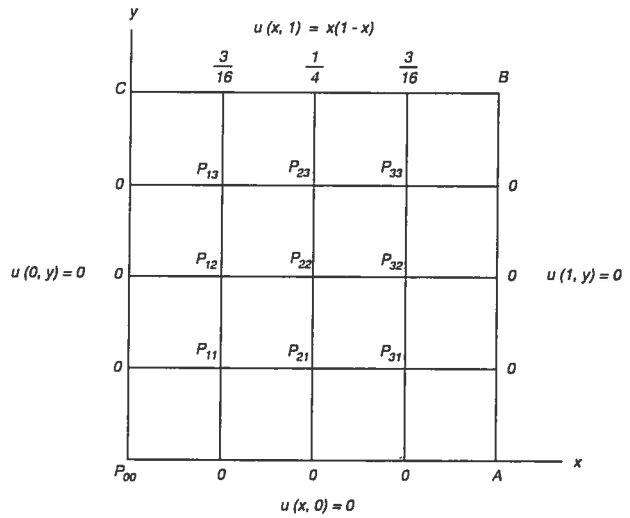

Figure 10.2 A typical lattice used in the approximate solution of Laplace's equation in the unit square. Source: Wylie and Barrett, 1982.

There is another way in which the finite-difference approximation to the Laplacian can be used to determine the value of the solution at the points of the grid. It is a simple iterative method, which proceeds as follows. We first recall that the finite-difference approximation to the Laplacian [Eq. (10.18)] expresses the value of the solution at any mesh point as the average of the values at the four adjacent points. Thus, after an initial estimate for the value of the solution at each mesh point has been made, they can be corrected and improved by systematically moving through the grid and replacing each value according to Eq. (10.18). In doing this, each value, as soon as it is corrected, should be used in all subsequent calculations.

As an illustration of this method, let us reconsider the problem we have just worked. Beginning with the estimates shown in Figure 10.3a, we have for the first refinement of u_{13} the value

$$u_{13} = \frac{0.1875 + 0.0000 + 0.1200 + 0.0600}{4} = 0.0919$$

Continuing through the grid as indicated using the corrected values as soon as they become available (but taking no advantage of the symmetry of the problem), we obtain the values shown in Figure 10.3b. Values bearing the subscript 1 were obtained by a single iteration; values bearing the subscript 5 were obtained after five iterations.

Parabolic Equations (The One-Dimensional Heat Equation). For the 1-D transport equation,

$$\frac{\partial^2 c}{\partial x^2} = a^2 \frac{\partial c}{\partial t} \tag{10.25}$$

the region of the x–t plane over which a solution is sought is always infinite, because of the infinite increase of time. As a finite-difference approximation to Eq. (10.25) we have, using Eqs. (10.13) and (10.14),

$$\frac{1}{h^2}(c_{i+1,j} - 2c_{i,j} + c_{i-1,j}) = \frac{a^2}{k}(c_{i,j+1} - c_{i,j}) \tag{10.26}$$

or, setting $m = k/a^2h^2$ and solving for $c_{i,j+1}$,

$$c_{i,j+1} = mc_{i+1,j} + (1-2m)c_{i,j} + mc_{i-1,j} \tag{10.27}$$

Clearly, it would be convenient to choose h and k so that the value of m is 1/2. The values of c on the boundary are of course provided by the data of the problem. Thus the given initial condition $c(x,0)$ provides the values of c_{00}, c_{10}, c_{20}, ... Similarly, end conditions of the form

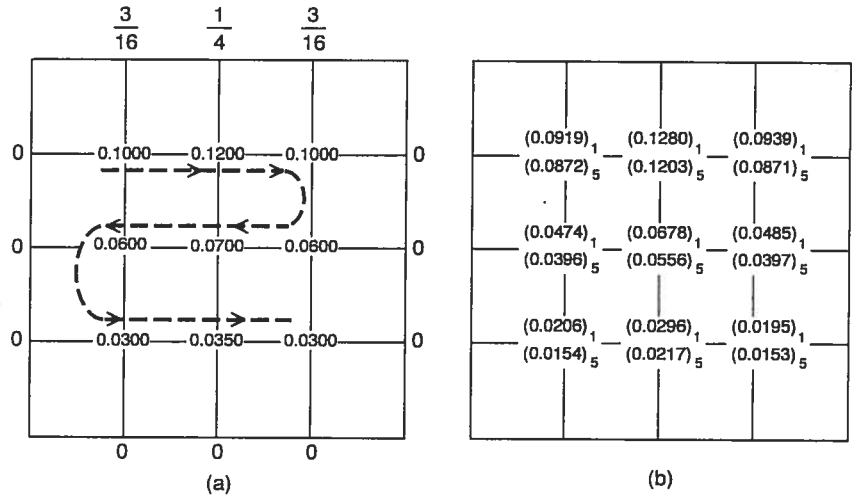

Figure 10.3 Data from an iterative solution of Laplace's equation. Source: Wylie and Barrett, 1982.

$$c(0,t) = g_1(t), \qquad c(l,t) = g_2(t) \tag{10.28}$$

where g_1 and g_2 are usually, though not necessarily, constant, furnish the values of c_{01}, c_{02}, c_{03}, ... and c_{l1}, c_{l2}, c_{l3}, ... No flow boundary conditions can, of course, be handled as outlined above in the discussion of Laplace's equation.

The determination of the solution over the rest of the grid proceeds in a straightforward way, using the extrapolation pattern provided by Eq. (10.26). First, the values of c_{11}, c_{21}, ..., $c_{l-1,1}$ are calculated from the known values of c_{00}, c_{10}, c_{20}, ..., c_{l0}. Then using these new values and the boundary values c_{01} and c_{l1}, the solution is "marched" forward by calculating the values of c at the grid points in the third row, and so on for the remainder of the grid.

10.3 FINITE DIFFERENCE METHODS

In general, a finite difference model is developed by superimposing a system of nodal points over the problem domain. In the finite difference method, nodes may be located inside cells (block-centered, Figure 10.4) or at the intersection of grid lines (mesh centered, Figure 10.5). Aquifer properties and head values are assumed to be constant within each cell in a block-

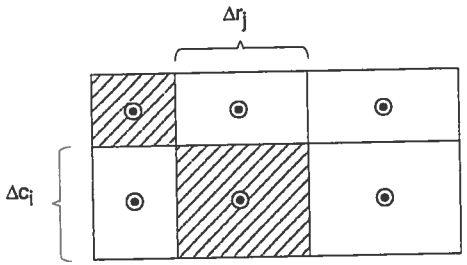

Figure 10.4 Block-centered grid system.

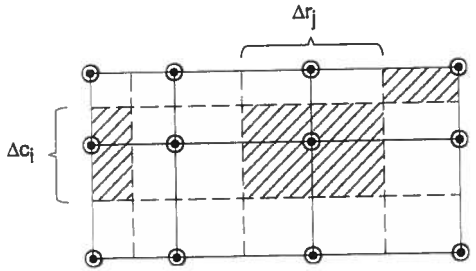

Figure 10.5 Point or mesh-centered grid system.

centered finite difference model. An equation is written in terms of each nodal point in finite difference models because the area surrounding a node is not directly involved in the development of the finite difference equations (Wang and Anderson, 1982).

The principles behind finite difference approximations will be illustrated using Laplace's equation in two dimensions:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = 0 \tag{10.29}$$

Consider a finite set of points on a regularly spaced grid (Figure 10.6). In the finite difference approximation, derivatives are replaced by differences taken between nodal points. A central approximation to $\partial^2 h/\partial x^2$ at (x_0, y_0) is obtained by approximating the first derivative at $(x_0 + \Delta x/2, y_0)$ and at $(x_0 - \Delta x/2, y_0)$ and then obtaining the second derivative by taking a difference between the first derivatives at those points

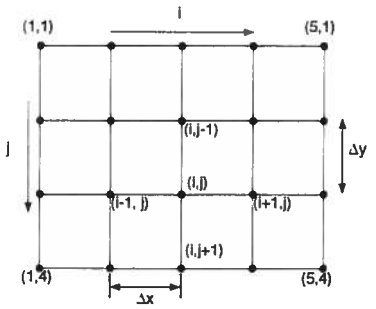

Figure 10.6 Finite-difference grid system.

$$\frac{\partial^2 h}{\partial x^2} \approx \frac{\dfrac{h_{i+1,j} - h_{i,j}}{\Delta x} - \dfrac{h_{i,j} - h_{i-1,j}}{\Delta x}}{\Delta x} \tag{10.30}$$

which simplifies to

$$\frac{\partial^2 h}{\partial x^2} \approx \frac{h_{i-1,j} - 2h_{i,j} + h_{i+1,j}}{\Delta x^2} \tag{10.31}$$

Similarly,

$$\frac{\partial^2 h}{\partial y^2} \approx \frac{h_{i,j-1} - 2h_{i,j} + h_{i,j+1}}{\Delta y^2} \tag{10.32}$$

By adding the expressions in Eqs. (10.31) and (10.32), and assuming that $\Delta x = \Delta y$, we obtain the finite difference approximation to Laplace's equation:

$$h_{i-1,j} + h_{i+1,j} + h_{i,j-1} + h_{i,j+1} - 4h_{i,j} = 0 \tag{10.33}$$

The generalized form of Eq. (10.33) is the most widely used equation in finite difference solutions of steady-state problems. There will be one equation of the form of Eq. (10.33) for each interior point (i,j) of the problem.

10.3.1 Explicit Finite Difference Approximation

For transient conditions, the head in an aquifer is a function of time; therefore, in addition to the spatial finite difference approximation for head, a finite difference approximation for $\partial h / \partial t$ is also needed. An **explicit** finite difference approximation is one where $h_{i,j}^{n+1}$ is calculated using only values of h known at time n. Explicit formulations are easily solved, because there is only one unknown variable in each equation. An explicit, **forward** difference approximation is given by

$$\frac{\partial h}{\partial t} \approx \frac{h_{i,j}^{n+1} - h_{i,j}^{n}}{\Delta t} \tag{10.34}$$

where n and $n+1$ represent two consecutive time levels. Similarly, an explicit, **backward** difference approximation is given by

$$\frac{\partial h}{\partial t} \approx \frac{h_{i,j}^{n} - h_{i,j}^{n-1}}{\Delta t} \tag{10.35}$$

Finally, an explicit, **central** difference approximation in time is given by

$$\frac{\partial h}{\partial t} \approx \frac{h_{i,j}^{n+1} - h_{i,j}^{n-1}}{2\Delta t} \tag{10.36}$$

The central difference approximation was found to be unconditionally unstable by Remson et al. (1971) and therefore should be avoided. For the case of transient flow, given by

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S}{T}\frac{\partial h}{\partial t} \tag{10.37}$$

an explicit approximation yields a stable solution if the value of the ratio $(T\Delta t)/[S(\Delta x)^2]$ is kept sufficiently small. In the 1-D case where flow occurs only in the x direction, the parameter $(T\Delta t)/[S(\Delta x)^2]$ must be ≤ 0.5 (Remson et al., 1971) to ensure numerical stability. For the 2-D case where $\Delta x = \Delta y = a$, $(T\Delta t)/[S(\Delta x)^2]$ must be ≤ 0.25 (Rushton and Redshaw, 1979).

10.3.2 Implicit Finite Difference Approximation

An **implicit** finite difference formulation is one where the heads h at time $n+1$ are evaluated using other values of head at time $n+1$. The solution to an implicit finite difference approximation involves a matrix of equations that must be solved simultaneously, because

there are several unknown variables in each equation. Implicit formulations will often use a weighted average of the approximations at n and $n+1$. The weighting parameter is represented by α, and it lies between 0 and 1. If the time step $n+1$ is weighted by α and time step n is weighted by $(1-\alpha)$, then:

$$\frac{\partial^2 h}{\partial x^2} \approx \alpha \frac{h_{i+1,j}^{n+1} - 2h_{i,j}^{n+1} + h_{i-1,j}^{n+1}}{(\Delta x)^2} + (1-\alpha)\frac{h_{i+1,j}^{n} - 2h_{i,j}^{n} + h_{i-1,j}^{n}}{(\Delta x)^2} \tag{10.38}$$

A similar expression is written for $\partial^2 h / \partial y^2$. The parameter α is selected by the modeler. For $\alpha = 1$, the space derivatives are approximated at $n+1$, and the finite difference scheme is said to be fully implicit. If a value of 0.5 is selected for α, then the scheme is referred to as the **Crank-Nicolson method.**

10.3.3 Alternating Direction Implicit (ADI)

The derivation and solution of the finite-difference equation and the use of the iterative ADI have been discussed extensively by Pinder and Bredehoeft (1968), Prickett and Lonnquist (1971), and Trescott et al. (1976). In general, the basis of the ADI method is to obtain a solution to the flow equation by alternately writing the finite-difference equation, first implicitly along columns and explicitly along rows, and then vice versa. In order to reduce the errors that may result from the ADI method, an iterative procedure is added so that within a single time step, the solution would converge within a specified error tolerance. The ADI method will be illustrated by approximating the 2-D transient equation for a confined aquifer:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S}{T}\frac{\partial h}{\partial t} \tag{10.39}$$

where S is the storage coefficient and T is the transmissivity. Assuming $\Delta x = \Delta y = a$, the fully implicit finite difference approximation is:

$$h_{i+1,j}^{n+1} + h_{i-1,j}^{n+1} + h_{i,j+1}^{n+1} + h_{i,j-1}^{n+1} - 4h_{i,j}^{n+1} = \frac{Sa^2}{T}\frac{h_{i,j}^{n+1} - h_{i,j}^{n}}{\Delta t} \tag{10.40}$$

In the first step of ADI, Eq. (10.40) is rewritten such that heads along columns are on one side of the equation and heads along rows are on the other side (also referred to as rewriting the equation, first implicitly along columns and explicitly along rows) results in:

$$h_{i,j-1}^{n+1} + \left(-4 - \frac{Sa^2}{T\Delta t}\right)h_{i,j}^{n+1} + h_{i,j+1}^{n+1} = -\frac{Sa^2}{T\Delta t}h_{i,j}^{n} - h_{i+1,j}^{n} - h_{i-1,j}^{n} \tag{10.41}$$

Eq. (10.41) will yield a tridiagonal coefficient matrix (one that has nonzero entries only along the three center diagonals) along any column (see Example 10.2). The second step of ADI involves rewriting Eq. (10.40) implicitly along rows and explicitly along columns:

$$h_{i-1,j}^{n+1} + \left(-4 - \frac{Sa^2}{T\Delta t}\right) h_{i,j}^{n+1} + h_{i+1,j}^{n+1} = -\frac{Sa^2}{T\Delta t} h_{i,j}^{n} - h_{i,j+1}^{n} - h_{i,j-1}^{n} \tag{10.42}$$

The explicit approximation along columns uncouples one row from another. Therefore, Eq. (10.42) will also generate a set of matrix equations—one for each interior row—with tridiagonal coefficient matrices. Alternating the explicit approximation between columns and rows is an attempt to compensate for errors generated in either direction.

10.3.4 Iterative Methods

A set of simultaneous finite difference equations could be solved directly; however, in problems having a large number of nodes, simultaneous solutions are impractical. Instead, iterative procedures can be used where an initial guess of the solution is made. Further improvements on the initial guess are then calculated. There are three commonly used iterative techniques: the **Jacobi iteration, Gauss-Seidel iteration,** and **Successive Over Relaxation (SOR).** Of the three, Jacobi iteration is the least efficient and Successive over relaxation is the most efficient.

Jacobi iteration. If Eq. (10.33) were solved for $h_{i,j}$, then:

$$h_{i,j} = \frac{h_{i-1,j} + h_{i+1,j} + h_{i,j-1} + h_{i,j+1}}{4} \tag{10.43}$$

The value of $h_{i,j}$ at any point is the average value of head computed from its four nearest neighbors.

The Jacobi iteration associates an **iteration index (m)** with the finite difference equation for head:

$$h_{i,j}^{m+1} = \frac{h_{i-1,j}^{m} + h_{i+1,j}^{m} + h_{i,j-1}^{m} + h_{i,j+1}^{m}}{4} \tag{10.44}$$

For $m = 1$, an initial guess of $h_{2,2}^{1}$, $h_{3,2}^{1}$, $h_{2,3}^{1}$, and $h_{3,3}^{1}$ is made. Eq. (10.44) is used to calculate head values for $m = 2, 3, \ldots, n$. Iteration continues until the solution converges to the preset error tolerance level, that is, the difference between the answers for $m = n$ and m = $n+1$ is less than the convergence criterion.

Gauss-Seidel iteration. The Gauss-Seidel iteration formula is:

$$h_{i,j}^{m+1} = \frac{h_{i-1,j}^{m+1} + h_{i,j-1}^{m+1} + h_{i+1,j}^{m+1} + h_{i,j+1}^{m+1}}{4} \tag{10.45}$$

Successive Over Relaxation (SOR). The SOR iteration is tied to the residual (c) or change between two successive Gauss-Seidel iterations:

$$c = h_{i,j}^{m+1} - h_{i,j}^{m} \tag{10.46}$$

The Gauss-Seidel iteration eliminates or **relaxes** the residual (c) by replacing $h_{i,j}^{m}$ with $h_{i,j}^{m+1}$ after each calculation. In the SOR method, on the other hand, the residual is multiplied by a relaxation factor ω, where $\omega \geq 1$. The value of $h_{i,j}^{m+1}$ is given by:

$$h_{i,j}^{m+1} = h_{i,j}^{m} + \omega c \tag{10.47}$$

A value of ω between 1 and 2 has been recommended (Wang and Anderson, 1982).

Example 10.2. TRIDIAGONAL MATRICES

Consider the 1-D transient flow equation:

$$\frac{\partial^2 h}{\partial x^2} = \frac{S}{T}\frac{\partial h}{\partial t} \tag{10.48}$$

The implicit or backward finite difference approximation, where the space derivative is evaluated at the $(n+1)$ time level, is

$$\frac{h_{i-1}^{n+1} - 2h_{i}^{n+1} + h_{i+1}^{n+1}}{(\Delta x)^2} = \frac{S}{T}\frac{h_{i}^{n+1} - h_{i}^{n}}{\Delta t} \tag{10.49}$$

Assume that we have a problem domain with six nodes where the first and last nodes are boundary nodes of known head. We wish to write the set of algebraic equations that would be generated by applying Eq. (10.49) to these nodes, and we wish to write it in matrix form.

Solution. First, we rearrange Eq. (10.49) and put unknowns, that is, heads at the $(n+1)$ time level, on the left-hand side and put knowns on the right-hand side.

$$h_{i-1}^{n+1} + \left(-2 - \frac{S(\Delta x)^2}{T\Delta t}\right) h_{i}^{n+1} + h_{i+1}^{n+1} = -\frac{S(\Delta x)^2}{T\Delta t} h_{i}^{n} \tag{10.50}$$

If the head values h_1 and h_6, which are known from the boundary conditions, are transferred to the right-hand side, then the matrix form of the set of algebraic equations for the six-node problem is

$$\begin{bmatrix} -2-\frac{S(\Delta x)^2}{T\Delta t} & 1 & 0 & 0 \\ 1 & -2-\frac{S(\Delta x)^2}{T\Delta t} & 1 & 0 \\ 0 & 1 & -2-\frac{S(\Delta x)^2}{T\Delta t} & 1 \\ 0 & 0 & 1 & -2-\frac{S(\Delta x)^2}{T\Delta t} \end{bmatrix} \begin{Bmatrix} h_2^{n+1} \\ h_3^{n+1} \\ h_4^{n+1} \\ h_5^{n+1} \end{Bmatrix} =$$

$$\begin{Bmatrix} -\frac{S(\Delta x)^2}{T\Delta t} & h_2^n - h_1 \\ -\frac{S(\Delta x)^2}{T\Delta t} & h_3^n \\ -\frac{S(\Delta x)^2}{T\Delta t} & h_4^n \\ -\frac{S(\Delta x)^2}{T\Delta t} & h_5^n - h_6 \end{Bmatrix}$$

The coefficient matrix has nonzero entries only along the three center diagonals. This type of matrix is known as a tridiagonal matrix, which is easily solved.

Example 10.3. FINITE DIFFERENCE APPROXIMATION TO THE DIFFUSION EQUATION

A finite difference approximation to the equation that describes steady-state diffusion of a dissolved substance into a quiescent fluid body in which a first-order reaction occurs has been derived by Celia and Gray (1992) as follows:

$$D\frac{d^2u}{dx^2} - Ku = 0 \qquad 0 < x < 1\ cm$$
$$u(0) = 0 \qquad u(1) = C_1 \tag{10.51}$$

where $u(x)$ [M/L^3] is the concentration of the dissolved substance, D [L^2/T] is the diffusion coefficient, K [1/T] is the reaction rate, and C_1 [L^2/T] is a specified concentration at the right boundary. The coefficients D, K, and C_1 are constants that, for this

calculation, will be assigned the following values: $D = 0.01$ cm^2/s, K=0.1 sec^{-1}, and $C_1 = 1.0$ g/cm^3.

The first step in deriving an approximate solution to Eq. (10.51) is the discretization step. First, three nodes are chosen, one at each boundary point and a third at $x = 0.5$. Thus three discrete values, (U_1, U_2, U_3), will be computed to approximate the true solution values $(u(0), u(0.5), u(1)) = (u_1, u_2, u_3)$. Because three unknowns are to be determined, three algebraic equations are needed. Two equations come directly from the boundary conditions, namely

$$U_1 = 0 \tag{10.52}$$

$$U_3 = C_1 \tag{10.53}$$

The finite difference approximation to the exact solution is thus required to exactly satisfy the first-type boundary (or Dirichlet) conditions. For all other nodes (in this case, only node 2), finite difference equations are written. Because the governing equation must hold at all points in the region $0 < x < 1$, it must be the case that the equation holds at $x = x_2 = 0.5$. Thus

$$D\left.\frac{d^2u}{dx^2}\right|_{x_2} - Ku|_{x_2} = 0$$

Taylor series expansion for the second derivative leads to the equality

$$D\left[\frac{u_1 - 2u_2 + u_3}{(\Delta x)^2} + \text{T.E.}\right] - Ku_2 = 0 \tag{10.54}$$

where T.E. is the truncation error, T.E., $u|_{x_2}$ is represented without error as u_2, and the constant spacing is denoted by Δx, with $\Delta x = 0.5$. Eq. (10.54) involves exact nodal values u_j $(j = 1,2,3)$. To write the appropriate finite difference approximation, the truncation error terms are neglected, resulting in the finite difference equation

$$D\frac{U_1 - 2U_2 + U_3}{(\Delta x)^2} - KU_2 = 0 \tag{10.55}$$

(Note that for this problem $U_1 = u_1$ and $U_3 = u_3$ while $U_2 = u_2$.) Eq. (10.55) is the algebraic equation used to solve for the nodal (finite difference) approximations U_j $(j = 1,2,3)$. Combination of Eqs. (10.52), (10.53) and (10.55) leads to

$$\begin{bmatrix} 1 & 0 & 0 \\ \frac{D}{(\Delta x)^2} & -K-\frac{2D}{(\Delta x)^2} & \frac{D}{(\Delta x)^2} \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ C_1 \end{bmatrix} \tag{10.56}$$

The solution of this set of equations is $U_1 = 0$, $U_2 = C_1 D/[2D + K(\Delta x)^2]$, $U_3 = C_1$. Using values of $D = 0.01$, $K = 0.1$, $C_1 = 1$, and $\Delta x = 0.5$, the solution is $U_2 = 0.222$. This compares to the exact solution $u(0.5) = 0.171$.

If four nodes are chosen instead such that $\Delta x = 1/3$, then the boundary conditions produce

$$U_1 = 0 \tag{10.57}$$

$$U_4 = 1 \tag{10.58}$$

and the two interior finite difference equations must be written, one corresponding to each interior node. The finite difference approximations analogous to Eq. (10.55) are

$$D\frac{U_1 - 2U_2 + U_3}{(\Delta x)^2} - KU_2 = 0 \tag{10.59}$$

$$D\frac{U_2 - 2U_3 + U_4}{(\Delta x)^2} - KU_3 = 0 \tag{10.60}$$

Given $\Delta x = 1/3$, and the previous values of D, K, and C_1, the approximation step produces the following set of linear algebraic equations:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0.09 & -0.28 & 0.09 & 0 \\ 0 & 0.09 & -0.28 & 0.09 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{10.61}$$

The solution step then produces the approximate solution $U = (0, 0.094, 0.291, 1)$; this compares to the analytical solution (0, 0.083, 0.320, 1).

Example 10.4. NUMERICAL SOLUTION FOR DRAWDOWN TO A WELL, TRANSIENT CONDITIONS

A FORTRAN program for solving the governing equation for drawdown to a well in a confined aquifer under transient conditions (Eq. 10.62) is available (Bedient and Huber, 1992). Assume T = 500 ft²/d and initial head = 20 ft. First, Eq. (10.62) can be written in finite difference form as

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = -\frac{R(x,y)}{T} \tag{10.62}$$

$$\alpha\left(\bar{h}_{i,j}^{n+1} - h_{i,j}^{n+1}\right) + (1-\alpha)\left(\bar{h}_{i,j}^{n} - h_{i,j}^{n}\right) = \frac{a^2 S}{4T}\frac{h_{i,j}^{n+1} - h_{i,j}^{n}}{\Delta t} - \frac{a^2 R_{i,j}^{n}}{4T} \tag{10.63}$$

where

$$\bar{h}_{i,j}{}^{n+1} = \frac{h^n{}_{i-1,j} + h^n{}_{i+1,j} + h^n{}_{i,j-1} + h^n{}_{i,j+1}}{4}$$

The iterative form of Eq. (10.63) is

$$h_{i,j}^{n+1} = \frac{\left[\alpha\bar{h}_{i,j}^{n+1}\right] + \frac{a^2 S}{4T\Delta t}h_{i,j}^{n} + (1-\alpha)\left[\bar{h}_{i,j}^{n} - h_{i,j}^{n} + \frac{a^2 R_{i,j}^{n}}{4T}\right]}{\frac{a^2 S}{4T\Delta t} + \alpha} \tag{10.64}$$

Assume that flow to the well in the aquifer described is transient. The well is pumping at a rate of 2500 ft³/d. If the storativity of the aquifer is 0.005, the drawdown near the well after one week can be determined. A starting time period of 0.05 days, a factor of 1.4 to increase the time increment (12 time iterations will equal about 7 days), the Crank-Nicolson scheme with $\alpha = 0.5$, a tolerance of 0.001, and no more than 200 iterations in the drawdown computation will be used for each time step. The computed drawdowns from the model are shown in Table 10.1. The solution can be compared

TABLE 10.1 Computed drawdown for Example 10.4

The Drawdown Array at Time = 6.96 is:									
0.88	0.88	0.87	0.85	0.82	0.80	0.78	0.76	0.75	0.74
0.90	0.89	0.88	0.86	0.83	0.81	0.78	0.76	0.75	0.75
0.93	0.93	0.91	0.89	0.86	0.83	0.80	0.78	0.76	0.76
1.00	0.99	0.97	0.93	0.90	0.86	0.82	0.80	0.78	0.78
1.10	1.09	1.05	1.00	0.95	0.90	0.86	0.83	0.81	0.80
1.24	1.22	1.16	1.09	1.02	0.95	0.90	0.86	0.83	0.82
1.45	1.40	1.30	1.19	1.09	1.00	0.93	0.89	0.86	0.85
1.76	1.65	1.47	1.30	1.16	1.05	0.97	0.91	0.88	0.87
2.32	1.98	1.65	1.40	1.22	1.09	0.99	0.93	0.89	0.88
3.56	2.32	1.76	1.45	1.25	1.10	1.00	0.94	0.90	0.89

TABLE 10.2 Comparison of Drawdown at 100 m from a Well using Numerical Solutions with Selected α and Theis Analytical Solutions

		Drawdown in Feet for			
Time (days)	Δt	α = 0	α = 0.5	α = 1	Theis
0.05	0.05	0.00	0.19 (4)	0.33(4)	0.011
0.12	0.07	0.68	1.03 (4)	1.28(5)	0.56
0.24	0.11	2.66	2.98 (5)	3.20(5)	3.00
0.41	0.17	6.57	6.41 (5)	6.37(6)	6.90
0.66	0.25	12.35	11.40 (6)	10.85(8)	11.82
1.04	0.38	18.95	17.54 (7)	16.43(10)	17.56
1.61	0.57	25.90	24.26 (9)	22.76(12)	23.79
2.46	0.85	32.60	31.21 (11)	29.52(16)	30.30
3.74	1.28	42.29	38.25 (14)	36.48(21)	37.06

The numbers in parentheses indicate the number of iterations used.

against the analytical Theis method at various points in time. It can be shown that the selection of Δx, Δy, Δt, and α will strongly influence the accuracy of the numerical results.

For the explicit case, if Δt is too large, the scheme becomes unstable and yields useless answers. Boundary conditions and choice of error tolerance in the iterative method also contribute to numerical errors. Results in Table 10.2 show the comparison of a numerical example with $Q = 1000$ m^3/day, $T = 4.50$ m^2/day, $S = 0.0005$, for various values of Δt and α. Values of $\Delta x = \Delta y = 100$ m were chosen. Theis results are also shown.

10.4 FINITE ELEMENT METHODS

One of the difficult problems in flow through porous media involves sharp fronts. A sharp front refers to a large change in a dependent variable over a small distance. Sharp front problems are encountered in both miscible (advective-dispersive flow) and immiscible (multifluid and multiphase flow) problems. The most common complaint about low order, finite-difference methods applied to sharp front problems is that the computed front is "smeared out." The process by which the front becomes smeared is referred to as **numerical dispersion.**

In general, for linear problems, the finite element method can track sharp fronts more accurately, which reduces considerably the numerical diffusion problem. The finite element

method, however, has several numerical problems, which include: numerical oscillation, instability, and large computation time requirements as will be seen later.

The finite element analysis of a physical problem can be described as follows (Huyakorn and Pinder, 1983):

1. The physical system is subdivided into a series of finite elements that are connected at a number of nodal points. Each element is identified by its element number and the lines connecting the nodal points situated on the boundaries of the element.
2. A matrix expression, known as the **element matrix**, is developed to relate the nodal variables of each element. The element matrix may be obtained via a mathematical formulation that makes use of either a variational or weighted residual method.
3. The element matrices are combined or assembled to form a set of algebraic equations that describe the entire system. The coefficient matrix of this final set of equations is called the global matrix.
4. Boundary conditions are incorporated into the global matrix equation.
5. The resulting set of simultaneous equations is solved using a variety of techniques such as the Gauss elimination.

Finite element methods will not be covered in this text.

10.5 METHOD OF CHARACTERISTICS (MOC)

The method of characteristics was developed by Garder et al. in 1964 mainly to overcome the numerical dispersion problem resulting from solving the advection-dispersion equation with conventional finite-difference techniques. The MOC has been widely used for simulating the transport of miscible compounds in ground water (Reddell and Sunada, 1970; Bredehoeft and Pinder, 1973; Konikow and Bredehoeft, 1974 and 1978).

The method of characteristics will be illustrated using the 1-D form of the transport equation for a conservative tracer:

$$D_x \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \tag{10.65}$$

where C is the tracer concentration, V is the velocity, D_x is the coefficient of hydrodynamic dispersion, and t is the time.

Equation (10.65) becomes hyperbolic as the dispersion term becomes small with respect to the advection term. The simplified set of equations in terms of an arbitrary curve

parameter is associated with the hyperbolic Eq. (10.65) is the MOC. Therefore, Eq. (10.65) can be simplified into the following system of Ordinary Differential Equations (ODEs):

$$\frac{dx}{dt} = V \tag{10.66}$$

$$\frac{dC}{dt} = D_x \frac{\partial^2 C}{\partial x^2} \tag{10.67}$$

The solutions of the simplified set of equations are called the characteristic curves of the differential equation. The numerical procedure proposed by Garder et al. (1964) involves both a stationary grid and a set of moving points. The stationary grid is obtained by subdividing the axis into intervals such that:

$$x_i = i\,\Delta x \quad \text{for} \quad i = 0, 1, ..., m-1 \tag{10.68}$$

A set of moving points or representative fluid particles with density of P points per grid interval is introduced into the numerical solution. The rate of change in concentration in the ground water is observed in the aquifer when moving with the fluid particle.

The location of each moving point is specified by its coordinate in the finite-difference grid. Initially, the moving points are uniformly distributed throughout the grid system. The initial concentration assigned to each point is the initial concentration associated with the interval containing the point. At each time interval, the moving points in the system are relocated in the flow field in proportion to the flow velocity at their respective location:

$$x_{p,n+1} = x_{p,n} + \Delta t_{n+1/2} V \tag{10.69}$$

where $x_{p,n+1}$, $x_{p,n}$ are the locations of particle p at time $n+1$ and n, respectively. After moving each point, the coordinates for the points are examined to determine in which interval the point lies. Each interval is assigned a concentration $C^*_{i,n}$ equal to the concentration of all the points that lie in the interval, after having been moved.

Next, the change in concentration due to dispersion is calculated for each interval:

$$\Delta C_{i,n+1/2} = \Delta t_{n+1/2} D_x \Delta x^2 C^*_{i,n} \tag{10.70}$$

Each moving point is then assigned a new concentration:

$$C_{p,n+1} = C_{p,n} + \Delta C_{i,n+1/2} \tag{10.71}$$

All points falling within an interval at a given time undergo the same change in concentration due to dispersion. Finally, the concentrations at the stationary grid points are computed for the new time step:

$$C_{i,n+1} = C^*_{i,n} + \Delta C_{i,n+1/2} \tag{10.72}$$

This completes the step from t_n to t_{n+1}, and the procedure is repeated for each subsequent time step.

Khaleel and Reddell (1986) provided listings of MOC programs for solving 1-D and 2-D tracer flow problems. They tested MOC for four cases: (1) longitudinal dispersion in 1-D flow; (2) longitudinal dispersion in 2-D flow; (3) longitudinal and lateral dispersion in 1-D flow; and (4) longitudinal and lateral dispersion in 2-D flow. For example, results from the 1-D MOC solution were compared to the analytical solution for the same problem provided by Ogata and Banks (1961) (see Chapter 6). Khaleel and Reddell's (1986) results showed good agreement between the analytical solution and the MOC numerical solution.

Similar results were obtained for the three other test cases. The reader is referred to the paper for more details on the test cases. It should be mentioned, however, that Khaleel and Reddell found it necessary to use a coordinate transformation to simulate 2-D flow fields more accurately. The coordinate axes were rotated so that an angle of 45° existed between the velocity vector and the transformed coordinate axes.

10.6 NUMERICAL FLOW MODELS

Computer models to simulate saturated ground water flow are typically 2-D or 3-D. Two-dimensional models may be used to simulate flow in the x-y plane or flow in a vertical cross section of the subsurface, and may simulate unsaturated or saturated water flow. Table 10.3 is a list of some of the available flow and contaminant transport models. Models that have seen extensive use include MOC and BIOPLUME II for 2-D contaminant transport with biodegradation (see Chapter 8). MT3D and RT3D are 3-D contaminant transport models that allow the user to incorporate reaction schemes. RT3D has been used to simulate chlorinated solvent reactions (Example 10.5). A detailed presentation of the MODFLOW model, one of the most widely used ground water flow models, serves to illustrate the main concepts involved in flow modeling.

TABLE 10.3 Selected Ground Water Flow and Contaminant Transport Models

Model Name	Model Description	Model Processes	Author(s)
BIOPLUME II (1987)	A two-dimensional model for simulating transport of a single dissolved hydrocarbon species under the influence of oxygen-limited biodegradation, first-order decay, linear sorption, advection, and dispersion.	decay dispersion advection adsorption	H.S. Rifai P.B. Bedient R.B. Borden J.F. Haasbeek
BIOPLUME III (1998)	Successor to BIOPLUME II. Two-dimensional model for reactive transport of multiple hydrocarbons under the influence of advection, dispersion, sorption, first-order decay, and reactant-limited biodegradation.	decay dispersion advection adsorption	H.S. Rifai C.J. Newell J.R. Gonzales S. Dendrou B. Dendrou L. Kennedy J.T. Wilson
CFEST (1987)	A three-dimensional finite-element model to simulate coupled transient flow, solute- and heat-transport in saturated porous media.	advection, dispersion diffusion, adsorption decay	S.K. Gupta C.T. Kinkaid P.R. Meyer C.A. Newbill C.R. Cole
FE3DGW (1985)	Transient or steady-state, finite-element three-dimensional simulation of flow in a large multi-layered groundwater basin.	leakage delayed yield compaction infiltration	S.K. Gupta C.R. Cole F.W. Bond
FEMWASTE/ FECWASTE (1981, 1987)	Two-dimensional transient finite-element model simulates areal or cross-sectional transport of dissolved constituents for a given velocity field in an anisotropic, heterogeneous porous medium	capillarity, convection dispersion, diffusion adsorption, decay	G.T. Yeh D.S. Ward
FLONET, FLOTRANS (1985)	Two-dimensional steady-state groundwater flow (FLONET) and transient solute transport (FLOTRANS) models for cross-sectional problems. FLOTRANS is an extension of FLONET.	decay, dispersion advection, adsorption	E.O. Frind
HELP (1987)	A water budget model for the Hydrologic Evaluation of Landfill Performance.	surface storage, runoff infiltration, percolation evapotranspiration, storage, soil moisture, lateral drainage	P.R. Schroeder J.M. Morgan T.M. Walski A.C. Gibson
MOC (1988)	To simulate transient, two-dimensional, horizontal ground water flow and solute transport in confined/ semiconfined aquifers using finite differences and method of characteristics.	advection, conduction dispersion, diffusion adsorption	L.F Konikow J.D. Bredehoeft

Table 10.3 Selected Ground Water Flow and Contaminant Transport Models (Continued)

Model Name	Model Description	Model Processes	Author(s)
MODFLOW (1988)	A modular three-dimensional finite-difference groundwater model to simulate transient flow in anisotropic, heterogeneous, layered aquifer systems.	evapotranspiration drainage	M.G. McDonald A.W. Harbaugh
MOTIF (1986)	Finite-element model for 1, 2, and 3-D saturated/unsaturated groundwater flow, heat transport, and solute transport in fractured porous media; facilitates single-species radionuclide transport and solute diffusion from fracture to rock matrix.	convection, dispersion diffusion, adsorption decay, advection	V. Guvanasen
MT3D (1990) MT3DMS (1998)	A three-dimensional transport model that uses flow fields. Particle tracking and finite difference methods are available to simulate anisotropic, heterogeneous, layered aquifer systems (MT3DMS is a multi-species update).	Advection, dispersion, sorption, decay	C. Zheng
Random Walk (1981)	To simulate one- or two-dimensional, steady/nonsteady flow and solute transport problems in a heterogeneous aquifer with water table and/or confined or semiconfined conditions, using a "random-walk" technique.	advection, dispersion diffusion, adsorption decay, chemical reaction	T.A. Prickett T.G. Naymik C.G. Lonnquist
RT3D (1998)	A three-dimensional reactive transport model. It uses the numerical engine of MT3D for multiple species and contains several pre-defined reaction schemes. User-defined reaction schemes can also be used.	Advection, dispersion, biodegradation, decay, sorption, monod, user-defined	T.P. Clement Y. Sun B.S. Hooker J.N. Petersen
SEFTRAN (1985)	A two-dimensional finite-element model for simulation of transient flow and transport of heat or solutes in anisotropic, heterogeneous porous media.	advection, dispersion diffusion, adsorption decay	P. Huyakorn
SUTRA (1984)	A finite-element simulation model for two-dimensional, transient or steady-state, saturated-unsaturated, density-dependent ground water flow with transport of energy or chemically reactive single species solutes.	capillarity, convection dispersion, diffusion adsorption, reactions	C.I. Voss
SWIFT II (1982)	A cross-sectional finite-element model for transient horizontal flow of salt and fresh water and analysis of upconing of an interface in a homogeneous aquifer.	buoyancy leakage	A. Verruijt J.B.S. Gan
USGS-3D-FLOW (1982)	A finite-difference model to simulate transient, three-dimensional and quasi-three-dimensional, saturated flow in anisotropic, heterogeneous groundwater systems.	evapotranspiration leakage	P.C. Trescott S.P. Larson

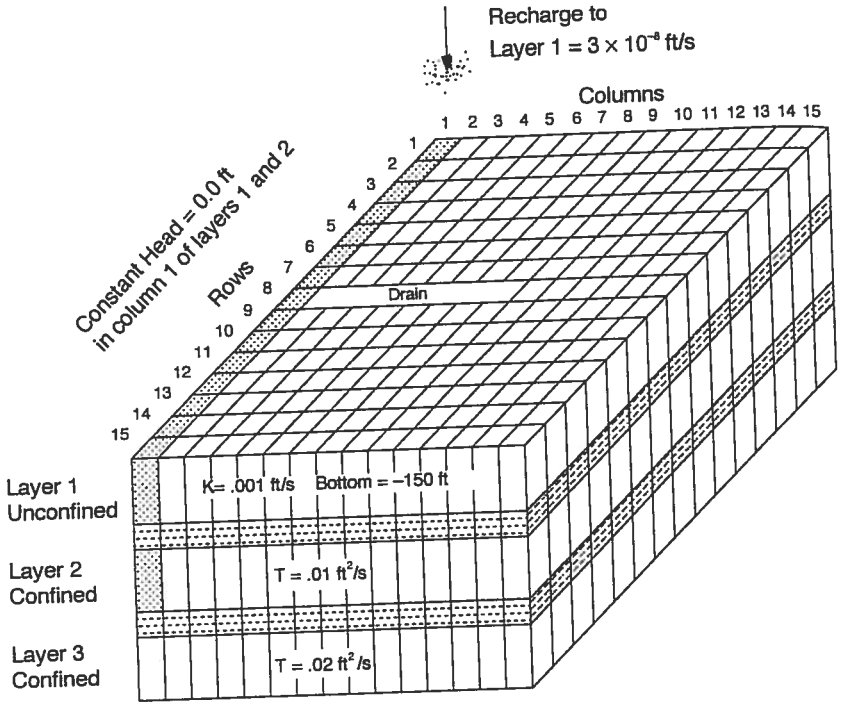

Figure 10.7 Schematic of an aquifer system in MODFLOW.

MODFLOW. MODFLOW, a modular 3-D finite-difference flow code developed by the U. S. Geological Survey (McDonald and Harbaugh, 1988), simulates saturated flow in three dimensions. It was designed such that the user can select a series of packages or modules to be used during a given simulation. Each module or package deals with a specific feature of the hydrologic system which is to be simulated, (e.g., wells, recharge, and rivers). The model contains several interdependent modules, of which the basic, block centered flow, and one of the three solution packages (strongly implicit, slice-successive overrelaxation, or pre-conditioned gradient) are required for every simulation.

MODFLOW can be used to simulate fully 3-D systems (Figure 10.7) and quasi three-dimensional systems in which the flow in aquifers is horizontal and flow through confining beds is vertical. The model can also be used in a two-dimensional mode for simulating flow in a single layer or two-dimensional flow in a vertical cross section. An aquifer can be confined, unconfined or a mixed confined/unconfined. Flow from external stresses, such as flow

to wells, areal recharge, evapotranspiration, flow to drains, and flow through riverbeds, can also be simulated.

For unconfined and mixed confined/unconfined aquifers, the elevations of the top and bottom of the aquifer are input and used in the model to calculate the saturated thickness based on the location of the water table within the aquifer. For confined aquifers, thickness is incorporated in the transmissivity distribution specified for the layers (Figure 10.7). Low-conductivity units or clay units are typically not included in the vertical discretization of the system, but rather are included through the use of a conductance term between the upper and lower units separated by the clay. Boundary conditions handled by the model include constant head, no flow and flux boundaries, and general head boundaries (in which a constant head is applied some distance from the edge of the model). Simulation time is divided into stress periods, which are in turn divided into time steps. A stress period is a time during which aquifer stresses (such as pumping and recharge rates) do not change. For transient simulations, the time steps may form a geometric series in which the parameters of the series, the number of time steps, and the multiplier are specified.

The primary output from the model is the head distribution. In addition, a volumetric water budget is provided as a check on the numerical accuracy of the simulation. The model was designed to provide a cell-by-cell flow distribution if required by the user. MODFLOW can also output a "head and flow file" which can be used by several transport models as described in the next section. An example is presented in section 10.8.

10.7 CONTAMINANT TRANSPORT MODELS

Many numerical transport models have been developed over the past 30 years. These models utilize a variety of numerical techniques and solve various forms of the governing transport equation, each subject to a certain set of boundary conditions. In addition, these models may simulate transport in one, two, or three dimensions; in the saturated or unsaturated zone; and miscible or immiscible transport. Table 10.3 provides a listing of some of these models. One should consult the International Ground Water Modeling Center (http://www.mines.edu/research/igwmc/) for other listings of available models. Additional information about modeling, and a listing of publicly available groundwater models is available at the US EPA's Center for Subsurface Modeling Support (http://www.epa.gov/ada/csmos.html), and the USGS's groundwater software information center at http://water.usgs.gov/software.

Reviewing each one of the contaminant transport models listed in Table 10.3 is beyond the scope of this chapter. One class of transport models, however, that is currently evolving and needs to be briefly mentioned is that of 3-D models which use the flow results of MODFLOW. These models use the same grid definitions defined for a MODFLOW run, and perform contaminant transport calculations with assigned sources, sinks, etc. They include:

- MODPATH (Pollock, 1988 and 1989)
- PATH3D (Zheng, 1989)
- MT3D (Zheng, 1990; Zheng, 1992)
- SEAM3D (Widdowson et al., 1997)
- RT3D (Clement, 1998),
- MT3DMS (Zheng and Wang, 1998)

In particular, SEAM3D, MT3DMS, and RT3D are all based on the MT3D engine, and offer similar multi-species contaminant transport support. The remainder of the section will focus on reviewing the MOC model, the MT3D model and MT3Ds successors in an effort to demonstrate the utility of ground water contaminant transport models.

10.7.1 USGS Two-Dimensional Solute Transport Model — MOC

The method of characteristics (MOC) is used in the USGS model to solve the solute transport equation (Figure 10.8). In order to apply the model to a field site, it is necessary to superimpose a block-centered finite-difference grid over the site by specifying the number of cells in the x and y directions (note that the y-axis should be oriented along the main direction of flow at the site). The values of the various parameters in the model can be uniform over the whole domain, or varying over each cell in the domain (see Section 10.5).

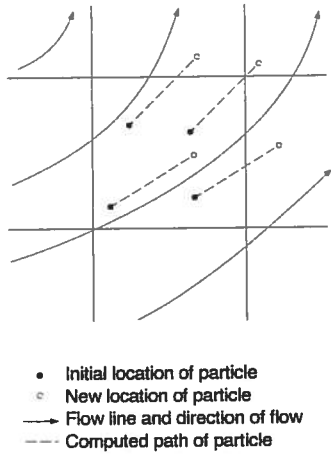

Figure 10.8 Particle tracking in USGS two-dimensional Model.

The finite-difference flow equation is solved numerically in MOC using an iterative alternating-direction implicit (ADI) procedure. The aquifer specific parameters in MOC include porosity, longitudinal and transverse dispersivity, thickness of the aquifer, transmissivity, and recharge. There are several model parameters that relate to the numerical methods used in MOC.

Two control parameters are used for the transport equation. The first parameter is used to limit the maximum distance within a cell that a particle can move during a time step. The time step is determined internally in the model and is controlled by four stability criteria that are discussed later in this section. The second parameter is the number of particles in a cell (up to 16). A related parameter is utilized to specify the maximum number of particles in the whole grid. The length of time for which modeling is required is specified in MOC using three parameters: the number of pumping periods in the simulation time, the actual time in years for each pumping period, and the number of time steps in a pumping period.

Source parameters include injection wells, constant concentration cells, and recharge cells. Injection wells and recharge cells basically define a source that leaks into an aquifer, that is, a source that has a flow rate and a concentration associated with it ($Q = Q_0$ and $C = C_0$). A constant concentration cell ($C = C_0$ boundary condition) simulates a source that adds contaminant mass at natural gradients into the aquifer. The MOC model allows the specification of up to five observation wells or monitoring wells at a given site. The history of chemical concentrations in those wells is included in the output from the model.

Boundary conditions in MOC are specified by the user. Types of boundary conditions that can be used include constant head cells or constant flux cells. A constant flux boundary can be used to represent aquifer underflow, well withdrawals, or well injection. A constant head boundary can represent parts of the aquifer where the head will not change in time. Constant head boundaries are simulated by using a high leakage term ($1.0\ s^{-1}$). The resulting rate of leakage into or out of the constant head cell would equal the flux required to maintain the head in the aquifer at the specified altitude. If a constant flux or constant head boundary represents a source, then the chemical concentration must be specified.

The numerical procedure in MOC requires that a no-flow boundary surrounds the modeled site. No-flow boundaries simply preclude the flow of water or contaminants across the boundaries of the cell. Initial conditions in the aquifer also have to be specified: the initial water table, and the initial contaminant concentrations.

The output from the MOC model consists generally of a head map and a chemical concentration map for each node in the grid. Immediately following the head and concentration maps is a listing of the hydraulic and transport errors. If observation wells had been specified, a concentration history for those wells would be included in the output. Detailed examples using BIOPLUME II and III, which are based on the MOC code, modified for biodegradation, are presented in Chapters 8 and 13.

10.7.2 MT3D: A Modular Three-Dimensional Transport Model

MT3D is a transport model that complements the MODFLOW flow simulation model. MT3D solves the advection-dispersion equation with first-order reaction and sorption, using flow fields calculated during a corresponding MODFLOW model run. THE MODEL requires an identical grid layout to MODFLOW, to ensure correspondence between the flow simulation and the transport simulation. Therefore, MT3D can simulate the same range of 2-D and 3-D scenarios as MODFLOW.

MT3D includes five packages that control various aspects of ground water contaminant transport. The basic package contains basic model information, including grid size, and timing information, and is required for all model runs. The advection package controls the solution scheme to be used. MT3D contains four different solution packages, including: Method of Characteristics (MOC), as described in **Section 10.5**; Modified Method of Characteristics (MMOC), a particle tracking method that combines 'backward' particle tracking with an interpolation scheme to reduce the computational burden of a simulation, but does not handle sharp fronts very well; Hybrid Method of Characteristics (HMOC), which combines the standard MOC and the MMOC methods, alternating back and forth depending on the presence of sharp concentration fronts; and Upstream Finite Difference, a nonparticle based method, similar to the forward-differencing scheme described in Section 10.3.

The dispersion package controls the amount of dispersion introduced by the model, while the source-sink mixing package controls sources and sinks of concentration due to wells, drains, recharge, rivers/streams, general head boundaries, and evapotranspiration. MT3D requires only the concentration information for these processes, as the flow characteristics of the sources/sinks are contained in the 'head and flow file' written by MODFLOW. The sources/sinks, however, must correspond to sources and sinks entered into the MODFLOW model. Finally, the reaction model controls radioactive decay or biodegradation that is treated as first-order decay, and sorption using the linear, Freundlich, or Langmuir models.

10.7.3 RT3D: Reactive Transport In 3 Dimensions

RT3D, developed at Battelle Laboratories, is the first and most widely known of the multi-species models which use the numerical engine developed in MT3D (Clement et al, 1998). RT3D is based on the 1997 version of MT3D (DOD Version 1.5), but has extended MT3Ds capabilities with the addition of several reaction packages. RT3D can accommodate multiple sorbed and aqueous phase species with any one of seven pre-defined reaction frameworks, or any other novel framework that the user may define. This allows, for example, natural attenuation processes or an active remediation to be evaluated, and simulations can be applied to modeling contaminants such as heavy metals, explosive, petroleum hydrocarbons, and/or chlorinated solvents. Most of the reactions modeled by RT3D are for simulation of various biodegradation processes.

RT3D's preprogrammed reaction packages include: Instantaneous aerobic decay of BTEX; Instantaneous degradation of BTEX using multiple electron acceptors; Kinetically limited hydrocarbon biodegradation using multiple electron acceptors; Rate-limited sorption reactions; Double Monod method; Sequential decay reactions

(PCE -> TCE -> DCE -> VC -> Ethene)

and an Aerobic/anaerobic model for PCE/TCE degradation.

RT3D is used in the modeling example which follows (**Example 10.5**) to simulate the sequential biotransformation of PCE at a typical dry cleaner site.

10.7.4 MT3DMS: Multiple-Species Version Of MT3D

MT3DMS includes several enhancements over MT3D, besides multiple species capabilities (Zheng & Wang, 1998). A new advection solver method, called the total variation diminishing scheme (TVD) is included, which allows the user to select from three different solution methods, depending on the requirements of the system being modeled. Other new features are a new implicit generalized conjugate gradient solution method, nonequilibrium sorption, and the multiple-species structure that will accommodate add-on reaction packages, such as those in RT3D or SEAM3D. MT3DMS does not contain any reaction packages in its basic distribution.

10.7.5 SEAM3D: Sequential Electron Acceptor Model for 3D

SEAM3D, developed with funding from the U.S. military, is designed to simulate subsurface transport of multiple solutes under the same aquifer conditions as MODFLOW and MT3D (Widdowson et al., 1997). It includes the following extensions: multiple electron acceptors are simulated (O_2, NO_3^-, Mn(IV), Fe(III), SO_4^{2-}, and CO_2), with biodegradation occurring in sequence, according to laboratory observations; biodegradation is accomplished following Monod kinetics; immobile nonaqueous phase liquid (NAPL) mass can be placed in any cell, and it will dissolve according to equilibrium assumptions. SEAM3D is based on the MT3D transport engine.

10.8 MODELING WITH GRAPHICAL PRE-PROCESSORS

One of the greatest advances in ground water modeling (and surface water modeling) in the last decade is the advent of the graphical pre- and post-processor. Several systems have been developed recently that allow the user to create a conceptual model of subsurface conditions which can then be used to export aquifer parameters into ground water flow and contaminant transport models, such as MODFLOW and MT3D. These systems aid the modeler by assisting in data management. They include the Groundwater Modeling System (GMS) created by

the Engineering Computer Graphics Laboratory at Brigham Young University (http://www.ecgl.byu.edu) for the Department of Defense (DoD), and Visual MODFLOW, created by Waterloo Hydrogeologic Software (http://www.flowpath.com). The authors will focus on GMS as an example of this type of software due its utility and general acceptance. The general functionality of the different packages is very similar.

The GMS package is divided into several modules, including the Map module, for creating conceptual models, and for working with observed data; the 3-D grid module, for working with MODFLOW, MT3D, and several other models based on MODFLOW, as well as other 3-D grid data sets; the 3-D scatter module for working with 3-D scatter data sets, such as concentrations and conductivities; the 2-D grid and scatter modules for working with 2-D scatter data and gridded data sets; the borehole module for working with borehole information, including cone penetrometer data; the triangular interconnected network module, for working with surfaces; the solid module for working with stratigraphy; and the 2-D and 3-D mesh modules for working with finite element meshes (which can be used to run finite element models, such as FEMWATER).

In order to create a MODFLOW/MT3D model of a field site, the user will need to create a conceptual model of the site. Often, this will involve importing a base map via an image or a CAD file. The base map can be "registered" to the coordinate system desired by the user by locating three known points on the map. After the base map has been imported, the user can import or hand-place other relevant information, such as boreholes, well locations and observed concentrations, and source zones. Much of this information can be entered into the conceptual model before a model grid has been created. This allows for greater flexibility in deciding what the optimal model grid will be, before the process of assigning values to specific grid cells begins, and allows the user to change grid definitions without losing the information entered into the grid.

GMS also offers several interpolation/extrapolation options for spatially variable data. For example, one might have hydraulic conductivity observations at several locations in the model area (from slug tests or pump tests). Using the interpolation methods (inverse distance weighted, nearest neighbor, kriging, etc.), the software will estimate the values for each point on the model grid. Data calculators are available to manipulate 2-D and 3-D data sets, with standard mathematical functions, as well as minimum, maximum, etc.

Once the model is built, the user can run MODFLOW, MT3D, RT3D, and other models directly from GMS, and read the output into GMS for post-analysis. Post-analysis can consist of drawing 2-D layer contours, taking cross sections, drawing 3-D contours, comparisons with observed data, and several other options. One of the major advantages of using an integrated pre- and post-processor is the ease of calibration of a model. The integration of observed data into the modeling system allows the user to compare model outputs with observed data in several ways, either through plotting contours of modeled and observed data, or by plotting *x-y* scatter plots of modeled versus observed values, in which a 45° angle represents a direct match, or by plotting a time series of observed and modeled concentrations for a single observation point (Holder et al., 1998).

Example 10.5 MODELING A DRY CLEANER SITE WITH GMS

GMS was used to create MODFLOW and RT3D models of a dry cleaner site in Houston, Texas, in which PCE contamination has impacted a local neighborhood. Contamination related to dry cleaning facilities has become an issue in the 1990s analogous to LPST releases in the 1980s. Dry cleaners are generally small and located near residential neighborhoods, making chemical discharges a serious health concern since the solvent used to dry clean, perchloroethylene (PCE) is a suspected carcinogen with a drinking water maximum contaminant level of 5 μg/L. Dry cleaners use 56% of the perchloroethylene in the United States (Izzo, 1992)

Aside from obvious contamination sources typically associated with any chemical operation, such as tank storage areas, process equipment, and loading docks, dry cleaners have additional sources that may contaminate the subsurface. Inadequate PCE recovery equipment may lead to PCE entering the sanitary sewer lines. PCE may then be released to the subsurface from flaws and joints in the piping, or by degrading certain types of polymer piping, such as ABS or PVC (Ranney and Parker, 1995). Many dry cleaners also have below ground lint traps, usually constructed from concrete. PCE may migrate through cracks in the concrete as well. Contamination from these sources may not be easily detectable and may constitute the bulk of the chemical release from the dry cleaner (See Figure 4.10).

PCE in the organic phase is a dense nonaqueous phase liquid (DNAPL), as described in Chapter 11, and will pass through the soil matrix, leaving small droplets of residual NAPL behind. As ground water sweeps through the aquifer, the PCE will slowly dissolve into the fresh ground water, with a solubility of about 150 mg/L. The residual PCE is a continuing source of contamination to the aquifer that may affect ground water quality long after the dry cleaner closes. The pools are difficult to find so it is generally accepted as a rule of thumb that if ground water concentrations greater than 1% of the aqueous solubility are detected, it is a strong possibility that a nonaqueous phase exists (Pankow and Cherry, 1996 and Chapter 11).

Two dry cleaner facilities were located in the contaminated area at the Houston site (Figure 10.9). The first operated from the mid-1970s until 1996, while the second opened in 1993 and is still in operation. Beneath the surficial clay in Houston, the affected aquifer is silty/sandy with a hydraulic conductivity of 5×10^{-3} cm/s. The aquifer is unconfined with the water table at about 20 ft below ground surface (BGS), and a clay layer approximately 30 - 35 ft BGS. The gradient of the ground water is approximately 0.005, in a generally southward direction. A stream north/northeast of the facilities provides shallow ground water recharge in the region.

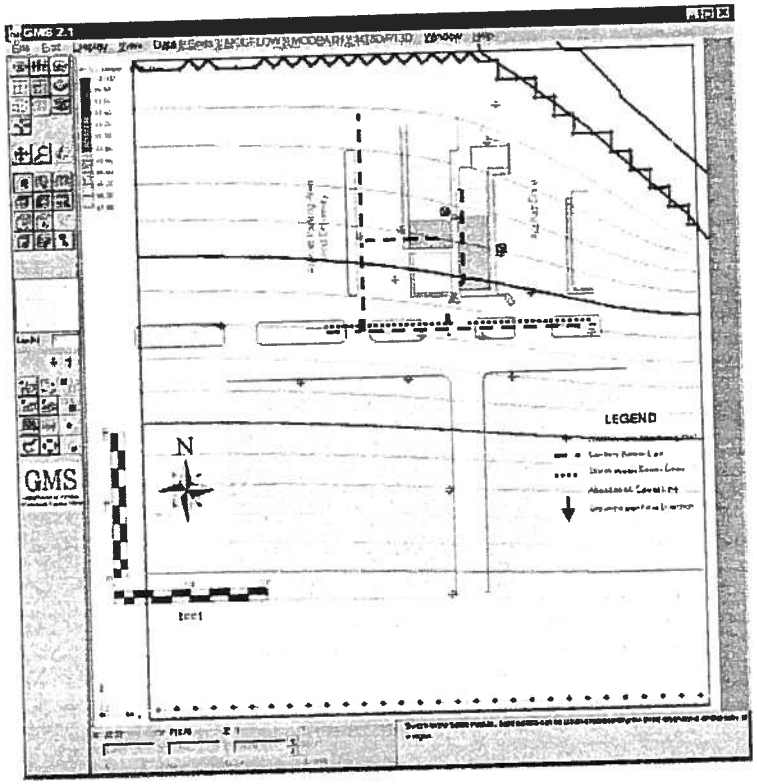

Figure 10.9 Ground water contours at two dry cleaner sites in Houston. The dry cleaners are the dark gray buildings.

Samples taken from the site show the primary concentration of the plume to be located in the area between the two cleaners. Contamination has moved off-site and migrated at least 2000 ft downgradient, and the plume is approximately 500 ft wide. The presence of TCE, the primary product of a PCE dechlorination, indicates that *in situ* biotransformation is occurring at this site. The site does not show direct evidence of a DNAPL since the maximum concentrations are less than the 1.5 mg/L rule of thumb (1% of 150 mg/L). However, the PCE concentrations are still much higher than the 5 μg/L limit needed to comply with drinking water standards.

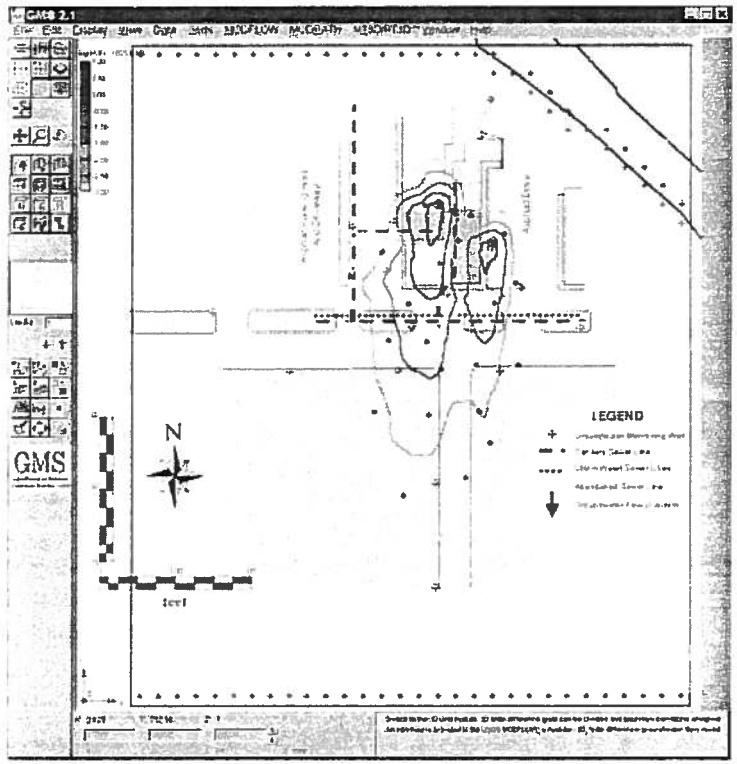

Figure 10.10 PCE concentrations modeled at the two dry cleaner sites.

The shallow aquifer characteristics were entered into the "map" module of GMS, along with two wells, representing sources of contamination at each site. Using resources such as site maps and USGS Digital Raster Graphics (DRGs) to locate relevant features, such as the stream, model boundaries were chosen, a grid was created, and the aquifer information from the map module was transferred to the MODFLOW and RT3D models. After the MODFLOW and RT3D models were created, they were checked with a built-in model checker, which looks for common modeling errors (e.g., zeros in the hydraulic conductivity field, etc.), and several model runs were performed. First, MODFLOW was run to get the head and flow values, which were checked against observed data. At this time, modifications needed to calibrate the flow modeling are done (see Section 10.9), then RT3D is run, using the heads and flows calculated in MODFLOW. Figure 10.10 shows the resulting PCE concentrations for 1998.

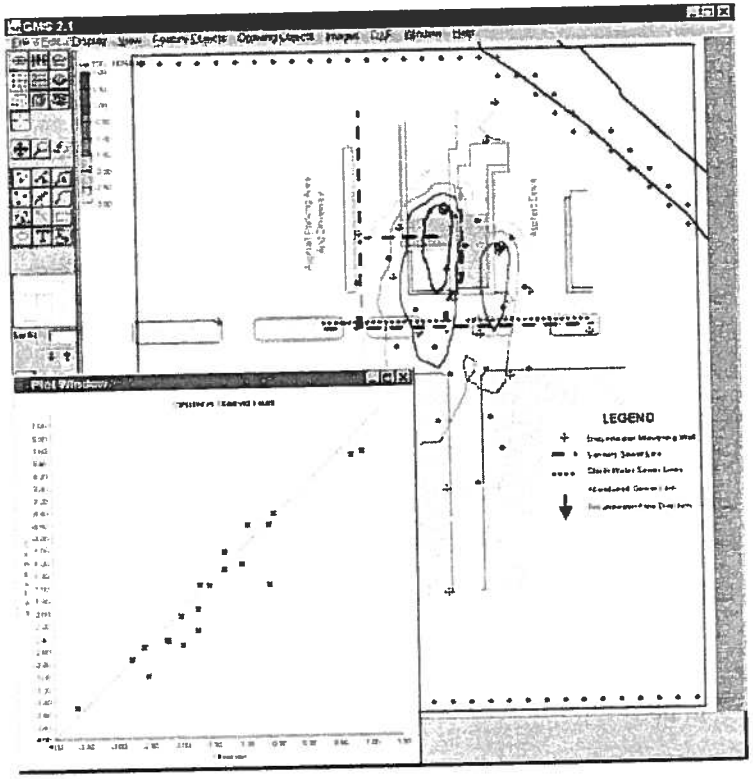

Figure 10.11 TCE concentrations at the dry cleaner sites, along with a calibration plot showing a comparison of computed v. measured data.

Several methods of comparison between modeled and observed values are possible. A visual comparison of contours can give a general sense of the plume size, maxima locations, etc. An x-y plot of modeled vs. observed data (Figure 10.11) provides a different comparison, which can be extremely useful in determining goodness of fit. From the general closeness of the data to the 45° line, the dry cleaner model fits the observed data reasonably well. Due to the wide variation in measured values of concentrations and hydraulic conductivities, it is often useful to plot these variables on a logarithmic scale, as shown in Figure 10.11. The logarithmic scale emphasizes the difference between measurements that span several orders of magnitude. In this case, using a linear scale would make concentrations of 0.001 mg/L and 0.1 mg/L almost indistinguishable.

The modeling of this site was made simpler and more effective using the pre- and post-processor GMS; which represents a significant improvement in time and effort over earlier methods in the 1980s. The calibration tools and the integrated visualization methods were used to help assure the model's accuracy. The prospective modeler must remember, however, that the accuracy and usefulness of a model are dependent on the available input data, and on the proper application of the modeling techniques described in Section 10.9.

10.9 APPLYING NUMERICAL MODELS TO FIELD SITES

Good field data are essential when using a model for simulating existing flow and/or contaminant conditions at a site or when using a model for predictive purposes. However, an attempt to model a system with insufficient data may be useful because it may serve as a method for identifying those areas where detailed field information needs to be collected. As mentioned earlier, a good modeling methodology will increase confidence in modeling results. In this section, emphasis is placed on outlining the procedure of designing and applying a selected ground water model to a field site. This step corresponds to item #4 in the modeling protocol established by Anderson and Woessner (1992), which was discussed in Section 10.1.

10.9.1 Model Set-Up

Once a conceptual model has been developed for the site and a computer model selected, it becomes necessary to interpret the conceptual model, and translate it into an input file that can then be used by the model. The interpretation process begins by analyzing the hydrogeologic and water quality data collected at the site, with the objective of predicting trends in the data and estimating the parameters required to run the model.

Data collection and analysis. Most site characterization efforts include identification of the subsurface geology, history of contamination, and water quality at the site. The stratigraphy is determined using soil borings, well logs, and geophysical tools. The subsurface geologic data usually has to be interpreted into values of the hydraulic conductivity and/or transmissivity, thickness of unit, and porosity, which can then be used as input to the model. The elevation of the water table and/or the potentiometric surface measured at discrete monitoring wells can be interpreted by constructing water level contours to determine the general direction of ground water flow.

Water quality data collected at specified time intervals from monitoring wells are generally analyzed to determine the trends in the spatial and temporal distributions of chemicals at the site. In many cases, the collected water quality data for a specific chemical are contoured to determine the extent of the plume of contamination.

For transport models, additional parameters that describe the physical, chemical, and biological properties of the chemicals of concern are necessary. A history of the chemical release (when it happened, how much was released) is an input requirement when one is attempting to simulate an existing contaminant plume. Defining whether a chemical is subject to biotic (or biological) and/or abiotic (chemical) reactions is essential for developing more representative models.

Parameter estimation. Obtaining the information necessary for modeling is not an easy task. Some data may be obtained from existing reports and studies, but more often it is necessary to rely on field characterization efforts. Transmissivity and the storage coefficient are typically obtained from pumping test results. Alternatively, the hydraulic conductivity is obtained from slug tests. For unconsolidated sands, the hydraulic conductivity may be obtained from laboratory grain size analyses or from permeability tests using permeameters.

Caution must be exercised when interpreting field measurements of hydraulic conductivity for use as input in ground water models. For instance, transmissivity values from pump tests are volume averaged; thus, the measured transmissivity is representative of the average properties of the aquifer zone influenced by the pump test. Hydraulic conductivity values, on the other hand, determined from slug tests are point values and only representative of the local zone where the slug test was conducted. Also, hydraulic conductivity values obtained from permeameter tests typically are several orders of magnitude smaller than values measured in situ.

Hydrologic stresses include pumping, recharge, and evapotranspiration. Of the three, pumping rates are the easiest to estimate. Recharge is one of the most difficult parameters to estimate. Recharge refers to the volume of infiltrated water that crosses the water table and becomes part of the ground water flow system (Anderson and Woessner, 1992). Discharge, on the other hand, refers to ground water that moves upward across the water table and discharges directly to the surface or the unsaturated zone. It is common for modelers to simulate recharge as a spatially uniform rate across the water table equal to some percentage of average annual precipitation. It is important to note, however, that this approach is very simplistic and does not take into account the spatial and temporal variations in recharge rates. Evapotranspiration may be determined from field measurements using lysimeters and/or studies of the vegetation.

10.9.2 Calibration

Calibrating a model is the process of demonstrating that the model is capable of producing field-measured values of the unknown model variable. For the case of ground water flow, for example, calibration is accomplished by finding a set of parameters, boundary and initial conditions, and stresses that produce simulated values of heads and/or fluxes that match measured values within a specified range of error.

Finding this set of parameter values has been compared by Anderson and Woessner (1992) to solving what is known as the **inverse problem**. In the ground water flow inverse problem, for instance, the objective is to determine values of the parameters from information about heads. The inverse problem contrasts with the forward problem, in which the specified model parameters are used to calculate heads.

There are two ways to achieve model calibration: (1) manual trial-and-error selection of parameters; and (2) automated parameter estimation. In trial-and-error calibration, parameter values are initially assigned to the grid. The initial parameter values are adjusted in sequential model runs to match simulated data to the calibration targets. Trial-and-error calibration may produce non-unique solutions because different combinations of parameters can yield essentially the same results. Also the trial-and-error process is quite subjective and is influenced by the modeler's expertise.

Automated inverse modeling may not be subjective and is not influenced by the modeler; however, it suffers from being complicated and computer intensive. Automated inverse modeling is also associated with instability problems and non-uniqueness in some cases. With the indirect approach, an inverse code automatically checks the head solution and adjusts parameters in a systematic way so as to minimize an objective function which compares the model calculated values of head to the measured values.

The results of the calibration should be evaluated relative to the measured values both qualitatively and quantitatively. To date, there is no standard protocol for evaluating model calibrations. A qualitative evaluation of the calibration involves comparing trends in the simulated results to those observed from the measured data. For example, a visual comparison could be made between contour maps of measured and simulated heads or concentrations to determine the similarities and differences between them. However, contour maps of field data themselves may include some error introduced by contouring and therefore should not be used as the only evaluation measure of calibration.

A quantitative evaluation of the calibration involves listing the measured and simulated values and determining some average of the algebraic differences between them. Two methods are commonly used to express this difference:

$$\text{Mean Error} = \frac{1}{n}\sum_{i=1}^{n}(x_m - x_s)_i \tag{10.94}$$

$$\text{Root Mean Squared Error} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_m - x_s)_i^2} \tag{10.95}$$

where x_m and x_s are the measured and simulated values, respectively.

10.9.3 Sensitivity Analysis

The purpose of a sensitivity analysis is to quantify the effects of uncertainty in the estimates of model parameters on model results. During a sensitivity analysis, calibrated values for

hydraulic conductivity, recharge, boundary conditions, etc., are systematically changed within a pre-established range of applicable values. The magnitude of change in heads and/or concentrations from the calibrated solution is a measure of the sensitivity of the solution to that particular parameter. The results of the sensitivity analysis are expressed as the effects of the parameter change on the average measurer of error (mean error or root mean square error) and on the spatial distribution of heads and/or concentrations.

10.9.4 Model Verification

Because of uncertainties in parameter estimates for a given site, the calibrated model parameters may not accurately represent the system under a different set of boundary conditions or hydrologic stresses. In a typical verification exercise, values of parameters and hydrologic stresses determined during calibration are used to simulate a transient response for which a set of field data exists (Anderson and Woessner, 1992). Examples of transient data sets include pumping test data and changes in water levels in response to pumping. In the absence of a transient data set, however, the model can be tested using a second set of steady-state data.

Unfortunately, sometimes it is not possible to verify a model because only one data set exists and it is usually used in the calibration process. A calibrated but unverified model can still be used to make predictions as long as sensitivity analyses of both the calibrated and predictive model are performed and evaluated.

10.9.5 Prediction

Prediction is one of the more common motivations for modeling. In a predictive simulation, the parameters determined during calibration are used to predict future conditions or the response of the system to future events. The length of time for which prediction may be required is an important consideration in model selection and design. For example, permitting for deep well injection of hazardous wastes requires contaminant transport modeling horizontally and vertically for 10,000 years. This implies that if a numerical model is used, care should be taken to ensure a large enough grid to allow for 10,000 years of transport.

The prediction process should be associated with a sensitivity analysis similar to that completed after calibration. Even though the calibrated model has been verified and subjected to a sensitivity analysis, the model may not give accurate results when stressed in some new way.

SUMMARY

Numerical models of groundwater flow and contaminant transport are designed to allow a modeler to simulate the groundwater conditions in an aquifer based on measurable aquifer and contaminant characteristics. The model is a mathematical representation of real-world physical, chemical, and/or biological processes, and can be used to predict future contamination, to interpret system dynamics, or to screen field sites for possible contamination problems. The mathematical representation is implemented using approximation techniques known as Finite Element, Finite Difference, or Method of Characteristics. An important part of modeling a site is the development of a conceptual model, which represents the parameters and processes that are important at the site. This conceptual model can be designed on paper or with the aid of new modeling software. The numerical model is assembled by interpreting information from the conceptual model.

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