System and Boundary Conceptualization in Ground-Water Flow Simulation

Techniques of Water-Resources Investigations of the United States Geological Survey

Book 3
Applications of Hydraulics

Chapter B8

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System and Boundary Conceptualization in Ground-Water Flow Simulation

By Thomas E. Reilly

Techniques of Water-Resources Investigations of the U.S. Geological Survey
Book 3, Applications of Hydraulics
Chapter B8

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CONVERSION FACTORS

Multiply	By	To obtain
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
square mile (mi^2)	2.590	square kilometer (km^2)
cubic foot per second (ft^3/s)	0.02832	cubic meter per second (m^3/s)
acre-foot (acre-ft)	4.356×10^4	cubic feet (ft^3)
acre-foot (acre-ft)	3.259×10^5	gallons (gal)

Metric units are used in all original work presented in this report. Two case studies are presented at the end of the report, however, that are based on previously published reports. The system of units that were originally used in these case studies are retained here in order not to introduce any round-off errors and to show the level of approximation used in the investigator’s estimates.

System and Boundary Conceptualization in Ground-Water Flow Simulation

By Thomas E. Reilly

ABSTRACT

Ground-water models attempt to represent an actual ground-water system with a mathematical counterpart. The conceptualization of how and where water originates in the ground-water-flow system and how and where it leaves the system is critical to the development of an accurate model. The mathematical representation of these boundaries in the model is important because many hydrologic boundary conditions can be mathematically represented in more than one way. The determination of which mathematical representation of a boundary condition is best usually is dependent upon the objectives of the study. This report focuses on the specific aspect of describing different ways to simulate, in a numerical model, the physical features that act as hydrologic boundaries in an actual ground-water system. The ramifications, benefits, and limitations of each approach are enumerated, and descriptions of the representation of boundaries in models for Long Island, New York, and the Middle Rio Grande Basin, New Mexico, illustrate the application of some of the methods.

INTRODUCTION

During the past several decades, computer simulation models for analyzing flow and solute transport in ground-water and surface-water systems have played an increasingly important role in the evaluation of alternative approaches to ground-water development and management. The use of these models has somewhat paralleled the widespread use of computers in today's society. Ground-water models (for example, McDonald and Harbaugh, 1988) attempt to represent the actual ground-water system with a mathematical counterpart. The underlying philosophy of the simulation approach is that an understanding of the basic laws of physics and an accurate description of the specific system under study will enable an accurate quantitative understanding of the cause and effect relationships. This quantitative understanding of these relationships enables forecasts to be made for any defined set of conditions, even those outside the range of observed conditions. Because of the uncertainties due to sparse or inaccurate data, poor definition of stresses, and errors in the scientists' deductive reasoning process, however, precise forecasts of future events will rarely be a reality for ground-water systems (see Konikow and Bredehoeft, 1992). Even though forecasts of future events based on models (if developed competently and objectively) are imprecise, they represent the best available decision making information at the time the forecasts are made.

Models that accurately represent the ground-water system being evaluated are expected to produce more accurate forecasts than those models that fail to represent important aspects of the system. The determination of which aspects of an actual ground-water system should be incorporated into a computer simulation usually depends, in part, upon the objectives of the study for which the model is being developed. The objectives of a study influence the size of the area of interest, the depth of concern, the scale of discretization (size of the model blocks or elements), and the method used to represent the boundary conditions of the model domain.

Computer simulations of ground-water flow systems numerically evaluate the mathematical equation governing the flow of fluids through porous media. This equation is a second-order partial differential equation with head as the dependent variable. In order to determine a unique solution of such a mathematical problem, it is necessary to specify boundary conditions around the flow domain for head (the dependent variable) or its derivatives (Collins, 1961). These mathematical problems are referred to as boundary-value problems. Thus, a requirement for the solution of the mathematical equation that describes ground-water flow is that boundary conditions must be prescribed over the boundary of the domain. Three types of boundary conditions – specified head, specified flow, and head-dependent flow – are commonly specified in mathematical analyses of ground-water flow systems (table 1). The values of head (the dependent function) in the flow domain must satisfy the pre-assigned boundary conditions to be a valid solution.

To obtain a solution to the ground-water flow equation, it is a mathematical requirement that boundary conditions be specified along the entire boundary of the three-dimensional flow domain. In solving a ground-water flow problem, however, the boundary conditions are not simply mathematical constraints; they generally represent the sources and sinks of

Table 1. Common designations for the three common mathematical boundary conditions specified in mathematical analyses of ground-water flow systems (Modified from Franke and others, 1987)
[h is head (L), n is directional coordinate normal to the boundary (L)]

Boundary type and name	Formal Name	Mathematical designation
Type 1 Specified head	Dirichlet	$h(x,y,z,t) = \text{constant}$
Type 2 Specified flow	Neumann	$\frac{dh(x,y,z,t)}{dn} = \text{constant}$
Type 3 Head-dependent flow	Cauchy	$\frac{dh}{dn} + ch = \text{constant}$ (where c is also a constant)

water within the system. Furthermore, their selection is critical to the development of an accurate model (Franke and others, 1987). Not only is the location of the boundaries important, but also their numerical or mathematical representation in the model. This is because many physical features that are hydrologic boundaries can be mathematically represented in more than one way. The determination of which mathematical representation of a boundary condition is best usually is dependent upon the objectives of the study. A model of a particular area developed for one study with a particular set of objectives may not necessarily be appropriate for another study in the same area, but with different objectives.

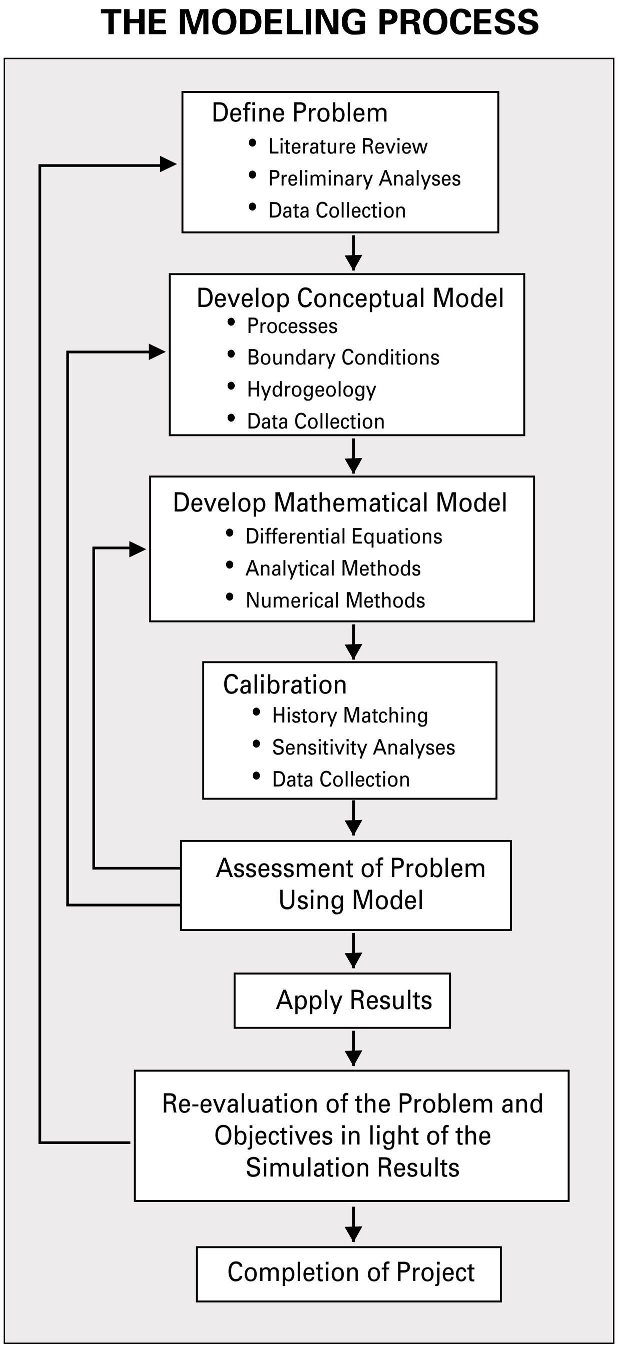


Figure 1. Flow chart of the ground-water flow modeling process.

Many reports and books have discussed the role and use of models in the analysis of ground-water problems (for example, Anderson and Woessner, 1992). Ground-water flow models attempt to represent the essential features and operation of the actual ground-water system by means of a mathematical counterpart. Figure 1 outlines some of the typical steps in the modeling process. One specific but very important component of the modeling process is the conceptualization and selection of boundary conditions, which is included as part of the second step called ‘Develop Conceptual Model’ in figure 1. Another important component is the mathematical approximation of hydrologic boundaries, which is included in the third step called ‘Develop Mathematical Model’ in figure 1.

Although some investigators have documented and explained the mathematical boundary conditions used in ground-water flow models (for example, Franke and others, 1987), most approach the topic from the applied mathematical perspective, which is based on the mathematical boundary types listed in table 1. This report attempts to use a physically based approach, using the physical features of the boundary surrounding the ground-water system as the focal point. The purpose of this report, then, is to focus on the specific aspect of boundary conditions in the modeling process by describing the different ways of simulating, in a numerical model, the physical features that are boundaries of the ground-water system, and to discuss the ramifications, benefits, and limitations of each approach. Careful conceptualization of the hydrologic system under study and a conscious selection of the best mathematical, or model, representation of the physical features that are hydrologic boundaries is a key to the development of reasonably accurate simulations.

SELECTION AND SIMULATION OF PHYSICAL FEATURES OF GROUND-WATER SYSTEMS AS BOUNDARY CONDITIONS IN GROUND-WATER FLOW MODELS

In the ground-water flow modeling process (fig. 1), boundary conditions have an important influence on the extent of the flow domain to be analyzed or simulated. In the problem definition stage, the extent of the flow domain is initially determined by the areal extent of the area of concern. In developing a conceptual model, the extent of the flow domain to be analyzed is expanded vertically and horizontally to coincide with physical features of the ground-water system that can be represented as boundaries. The effect of these boundaries on heads and flows must then be conceptualized, and the best or most appropriate mathematical representation of this effect is selected for use in the model. The key is to select the boundary of the model to coincide with a feature in the actual system that can be simulated reasonably well and that will minimize the effect of any artificial approximation. During the simulation process, the extent of the model, the conceptualization of the flow system, and mathematical representation of the boundaries is continually checked and evaluated to ensure the representation of the system captures the essence of the actual ground-water system.

A thorough understanding of hydrologic boundaries in nature and the different ways to simulate them is required to select the best mathematic representation in a ground-water flow model. The objective of the modeling analysis and the magnitude of the stresses to be simulated also influence the selection of the appropriate approach to simulate the physical features that bound the ground-water system. When ground-water systems are heavily stressed, the physical features that bound the system can change in response to the stress. Any representation of these features must account for these potential changes, either by understanding the limitations of the simulation or by representing the physical feature as realistically as possible.

This section of the report describes the various types of hydrologic boundaries that can affect ground-water flow systems. The different approaches that can be taken to simulate each physical feature are enumerated. The possible effects of each physical feature as a boundary on the flow system and the ramifications and limitations of the different approaches are discussed.

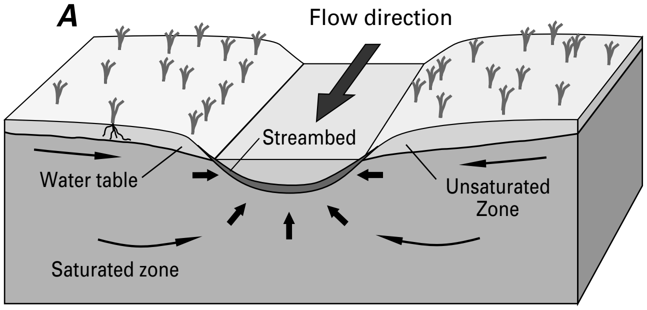
Streams

Streams are surface features that commonly form a boundary of the saturated ground-water flow system. Streams are important boundaries of ground-water systems because they influence the heads and flows of the ground-water system with which they interact. Streams can gain water from the ground-water system (fig. 2A) or lose water to the ground-water system (fig. 2B). Losing streams can be connected to the ground-water system by a continuous saturated zone (fig. 2B) or can be disconnected from the ground-water system by an unsaturated zone (fig. 2C). Some streambeds consist of material of low hydraulic conductivity that can cause a large head difference between the stream and the aquifer, while other streams may be well connected to the aquifer system through permeable material of high hydraulic conductivity. Some streams are deeply incised into the aquifer whereas others may not be.

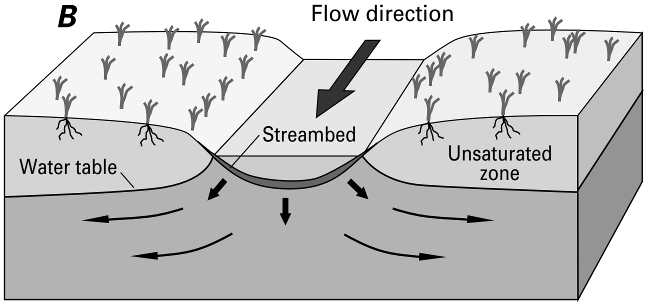
Just as there are many types of streams, there are many ways to represent a stream in a numerical model. Each way treats the interaction of the stream with the ground-water system differently. These different conceptualizations may produce the same results under some conditions and very different results under other conditions or stresses.

In ground-water models, a stream may be represented as:

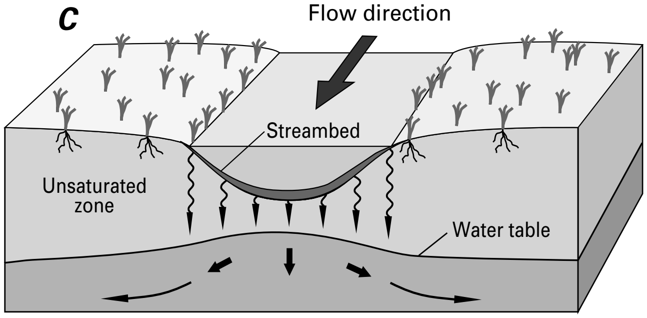
1. A specified-head boundary (also known as a Type 1 or Dirichlet boundary)
2. A specified-flow boundary (also known as a Type 2 or Neumann boundary)
3. A head-dependent or ‘leaky’ boundary (also known as a Type 3 or Cauchy boundary)
4. Nonlinear variations of the ‘leaky’ boundary:
    a. A strictly gaining stream (a drain)
    b. A stream with a constant stage that can become disconnected from the saturated zone
    c. A stream whose stage is calculated as part of the model solution.



GAINING STREAM



LOSING STREAM



LOSING STREAM THAT IS DISCONNECTED FROM THE WATER TABLE

Figure 2. Interactions of a stream and a ground-water system (Modified from Winter and others, 1998): (A) gaining stream, (B) losing stream, and (C) losing stream separated from the saturated ground-water system.

The level of complexity and data required varies for the different approaches. Each approach is valid for specific conceptualizations, and it is important that the type of boundary selected be consistent with the actual system, the objectives of the study, and the intended use of the model.

When a stream is represented as a specified-head boundary, nodes in the model, where the stream is located, are simulated with a head that is unchanging. This head, usually, is set at the stage of the stream. It implies that there is no head loss between the stream and the ground-water system and that the flow of ground water into or from the stream will not affect the stage of the stream (fig. 3A). The amount of water flowing between the stream and the ground-water system then depends upon the ground-water heads in the

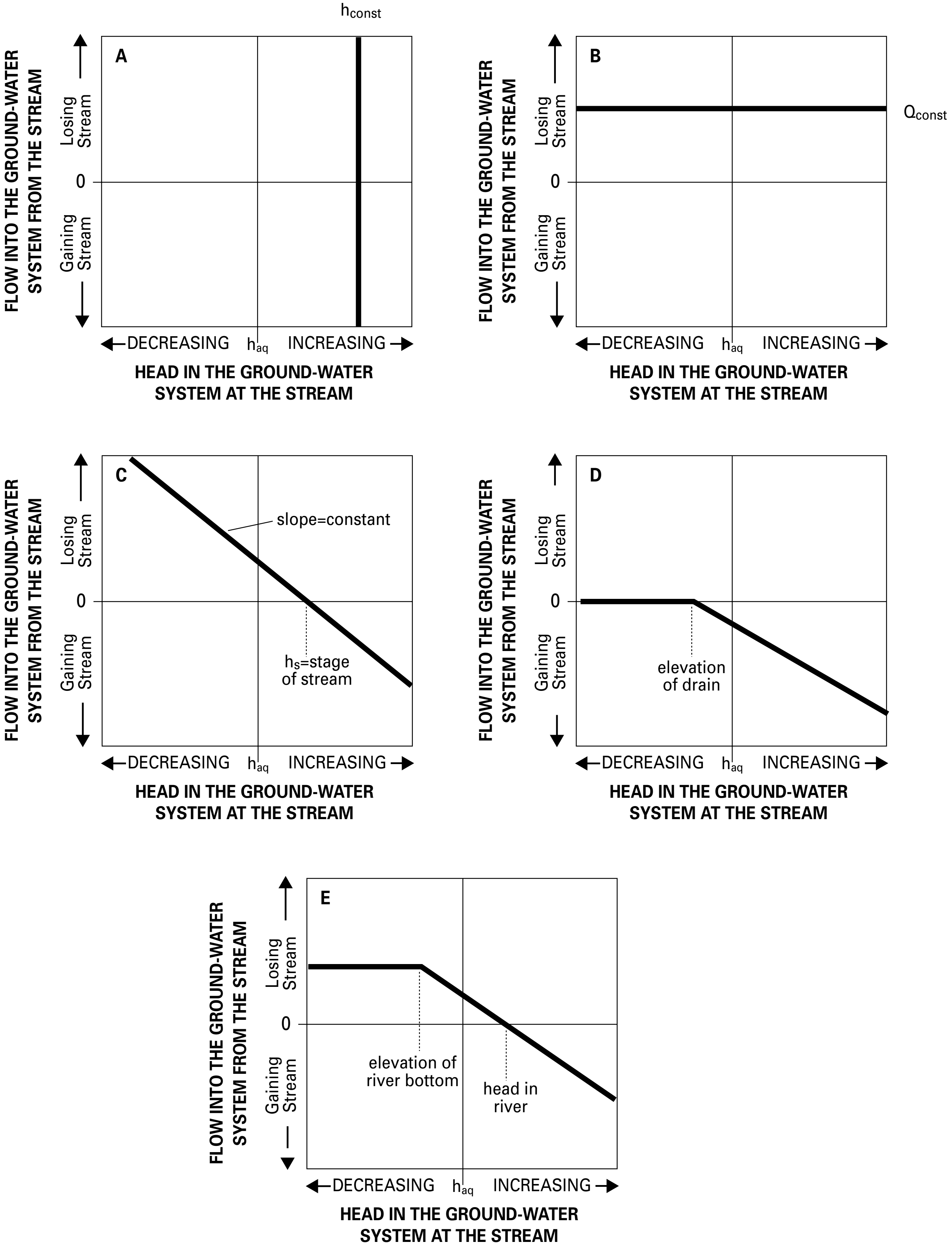


Figure 3. Relations between head and flow for different mathematical representations of the stream boundary: (A) constant head, (B) constant flow, (C) head-dependent flow, (D) limited head-dependent flow (drain), and (E) limited head-dependent flow (river).

nodes that surround the specified-head boundary representing the stream. This representation may be appropriate for large streams or for systems in which the stream is well connected to the ground-water system and the stream stage is not expected to change.

A stream can be simulated as a specified flow boundary if the loss or gain rate of the stream is known. This boundary is simulated by specifying a flow rate at a node or location representing the stream. In this representation, the flow rate is independent of the head in the aquifer (fig. 3B). This representation may be appropriate for streams that are disconnected from the ground-water system, such as streams at high altitudes that lose their water as they enter the valley deposits from the mountains. It also may be appropriate for some steady-state simulations of conditions in which the stream interaction has been well measured and no changes in stress will be simulated. Conceptually, representing the stream as a specified flow assumes that the flow of water between the ground water and the stream is independent of the heads in the ground-water system (fig. 3B) and the surface-water system.

A stream can be simulated as a head-dependent flow or 'leaky' boundary, which is also referred to as a 'general head boundary' in the finite-difference model MODFLOW (McDonald and Harbaugh, 1988). This boundary represents the stream as having a constant specified stage, but a layer of material (the streambed) or some other resistance is present between the stream and the ground-water system (fig. 4). This representation assumes that the stream and the ground-water system are always connected, and the flow from or to the stream is directly proportional to the head difference between the stream stage and the head in the ground-water system (fig. 3C).

The first three possible representations of a stream are all linear in that the stage in the stream and the equation representing the flow between the aquifer and the stream do not change as a function of the head in the ground-water system. Thus, these representations can be used in model conceptualizations that employ superposition (Reilly and others, 1987). The three remaining ways to represent a stream in a ground-water flow model are nonlinear variations of the 'leaky' boundary in that the coefficients of the equation used or the stage of the stream depends directly on the head in the aquifer.

The first representation, and perhaps the simplest of the nonlinear representations, is for the case of a strictly gaining stream. This case is simulated by use of the 'drain' package in MODFLOW (McDonald and Harbaugh, 1988). In this conceptualization, the only source of water to the stream or drain is that which enters the stream or drain as ground-water inflow. If the head in the ground-water system falls below the altitude of the stream or drain bottom, the ground-water inflow to the stream or drain ceases and the stream dries up (fig. 3D). This conceptualization is useful in simulating ground-water drains or headwater streams that have very little surface runoff relative to ground-water inflow. The representation of streams as a drain must be used cautiously, however, because each node represented as a drain is independent of all the other nodes represented as a drain. If a stream represented as a drain goes dry in the middle of its reach, it cannot represent the fact that water that is in the stream upstream from the dry section could infiltrate in the dry stream and provide flow from the stream to the aquifer. Thus, as with all boundary conceptualizations, the use of this conceptualization of a stream must be consistent with how the stream functions in nature.

The second representation (fig. 3E) is an extension of the 'leaky' boundary condition in that it also allows the head in the ground-water system to be below the stream bottom (fig. 2C). This case, for the condition in which the stream becomes disconnected from the ground-water system, is simulated as a condition of a fixed flow. When the stream becomes disconnected from the saturated ground-water system, the flow leaving the stream is independent of the head in the ground-water system. This representation assumes that the stage in the stream is specified and is not a function of the amount of ground-water inflow or outflow. Thus, the stream can never go dry regardless of how much water is lost to the ground-water system. When using this representation, the investigator must carefully examine the water budget of the system and of the boundary to ensure that the quantities of water being simulated in the model are plausible in the actual system.

The last representation is the most complex and can be implemented by many different means. For this last representation, a model of the stream system is coupled to the model of the ground-water system. In this approach, the stage of the stream is dependent upon the amount of flow in the stream and the amount of flow between the ground-water system and the stream. Existing models of stream systems are numerous and are based on different methods and levels of complexity. Three different methods for simulating a stream system have been implemented in the ground-water model MODFLOW. These are the stream-flow routing package (Prudic, 1989), DAFLOW-MODFLOW (Jobson and Harbaugh, 1999), and MODBRANCH (Swain and Wexler, 1993). These methods may represent the system accurately, but the information and data needs increase and the numeri-

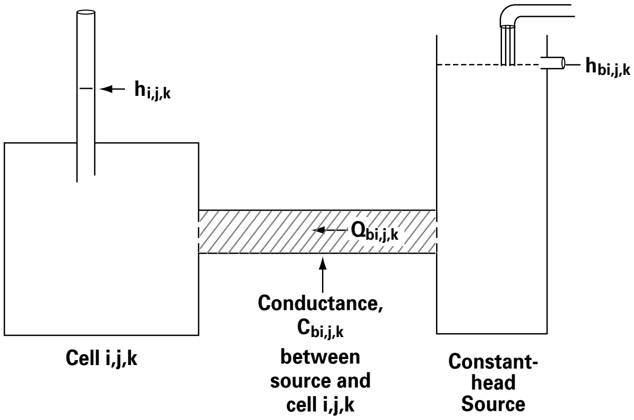


Figure 4. Conceptual representation of a head-dependent flow or 'leaky' boundary condition as implemented in a finite-difference flow model. (From McDonald and Harbaugh, 1988)

cal methods may lose stability for the more complex stream simulation packages. The response times for flow in streams is usually significantly faster than response times for ground-water systems and this incongruity can cause problems in determining an appropriate simulation strategy. This coupling of ground-water and surface-water models is needed where the short-term fluctuations in the ground-water system due to the influence of the surface water are important to the objectives of the study. The coupling of ground-water and surface-water models is also necessary if the stream may dry up or rewet during the course of the simulation. In cases in which this level of detail is not needed, the simpler methods can provide equivalent model results.

In model design, selection of the appropriate mathematical boundary condition to represent a particular stream in a hydrologic system is a key decision that can affect the ability of a model to make accurate forecasts. Considerations that must enter into the selection are the nature of the stream (for example, flow rate, variability of the flow, type of streambed, connection with the ground-water system), the objectives of the study, and the potential uses of the model. In methods that do not keep track of the amount of water in the stream, there are no constraints on the amount of water available from the stream. As pumping rates increase in such a system, an unrealistic amount of water may be induced to flow from the stream to the ground-water system. This means that the model user must check to see if the amount of water being supplied from the boundary (stream) is reasonable. For example, the simulated amount of water being supplied by the stream to the ground-water system should not exceed the total amount of streamflow available. Thus, the magnitude of the stress imposed on the system can affect the validity of the boundary condition. A model developed for one set of conditions may not be valid when applied to a different, more extreme set of conditions. The conceptualization of the interaction between the surface-water system and the ground-water system is very important and must be continually evaluated during the use of the model.

Lakes and Reservoirs

Lakes and reservoirs are usually hydraulically connected to ground-water flow systems and can be significant physical features of the flow system. The manner in which they are represented in a numerical model is important to accurately reproduce their role in the actual ground-water system. Their role is similar to that of streams in that lakes and reservoirs can lose water to the ground-water system, gain water from the ground-water system, or do both. In some situations, lakes and reservoirs can be simulated with the same boundary conditions as those used for streams. In some instances, however, where the lake or reservoir level and area are dependent upon the interaction with ground water, a more complex approach is required.

In ground-water models, a lake or reservoir may be represented as:

1. A specified-head boundary
2. A head-dependent or ‘leaky’ boundary
3. Nonlinear variations of the ‘leaky’ boundary:
   a. A lake or reservoir with a constant stage that can become disconnected from the saturated zone
   b. A lake or reservoir whose stage and area is problem dependent and is calculated as part of the model solution.
4. A volume of material of high hydraulic conductivity with recharge calculated as areal precipitation minus lake evaporation. (This is not strictly a boundary condition; rather it is an approach to simulate the effect of the lake.)

As with the simulation of streams, the appropriate method to simulate a lake or reservoir depends upon the characteristics of the lake or reservoir in nature (for example, size, stage variation, type of lake-bed sediments, sources of water) and the expected stresses to be imposed on the model (that is, the objectives of the study using the model).

For cases in which the lake or reservoir is large and no change in stage is expected for the stresses to be imposed on the model, the specified-head and head-dependent boundary conditions may be appropriate. As an example of this approach, Eberts and George (2000) represented Lake Erie as a specified-head boundary in their model of regional ground-water flow in the Midwestern Basins and Arches Aquifer System of Indiana, Ohio, Michigan, and Illinois. If the stage of the lake is dependent on the heads and flows in the ground-water system, however, then a different approach is required. For lakes with surface-water inflows and outflows, a model of the lake stage or lake area may be required. As examples of this approach, Cheng and Anderson (1993) used a formulation that calculated the lake stage as part of the model, Fenske and others (1996) used a formulation that calculated a changing area of infiltration for reservoirs for which the stage was prescribed over time, and Merritt and Konikow (2000) used a formulation that calculates both the stage and area of the lake as part of the model solution. For lakes that are basically surface expressions of the ground water system, the lake can be simulated as a volume of material of very high hydraulic conductivity with the recharge set at precipitation minus lake evaporation and a storage coefficient set at 1.0, as was implemented by Masterson and Barlow (1997) on Cape Cod, Mass.

A key to selecting the appropriate model representation of a lake or reservoir is to determine if the stresses to be analyzed during the model analysis will affect the stage (water level) in the lake or reservoir. If the stage will not be affected, then the simpler boundaries will suffice. The developer or user of the model must check this assumption by evaluating the changes in flow between the lake and the ground-water system to ensure that they can happen in the actual system without changes in stage occurring. For example, in a stressed system, if the flow from a lake into the ground-water system is larger than the amount of water flowing into the lake and recharging the lake, the lake level in the actual system cannot be supported and will have to change. These examples again point out that a model of a specific system is constructed by selecting boundary conditions based on certain assumptions regarding the use of the model, the amount of stress that will be simulated, and the accuracy required. If the model is used to evaluate conditions that no longer are the same as the design assumptions, the results will be invalid. It is important for the analyst to constantly evaluate the appropriateness of the methods used to simulate the boundary conditions during the use of the model.

Wetlands

Wetlands are present wherever topography and climate favor the accumulation or retention of water on the landscape. Wetlands occur in widely diverse settings, from coastal margins to flood plains to mountain valleys. Similar to streams, lakes, and reservoirs, wetlands can receive ground-water inflow, recharge ground water, or do both. A mathematical representation of a wetland would be the same or similar to the choices available for streams, lakes, and reservoirs. For example, Koreny and others (1999) represented a wetland that was known to recharge the underlying ground-water system as a specified inflow boundary. Winston (1996) used the ‘drain’ conceptualization in MODFLOW to represent a wetland that gained water from the ground-water system as a solely gaining discharge location. Swain and others (1996) used the MODFLOW/BRANCH model (Swain and Wexler, 1993) to represent wetlands in southern Dade County, Fla. as a highly permeable layer coupled to a surface-water model. The best representation should be based on an understanding of the source of water in the wetland and the factors that regulate the exchange of water between the ground-water system and the wetland. These factors are the same as those for streams, lakes, and reservoirs, and are described in the previous sections.

Springs

Springs typically are present where the water table intersects the land surface. Springs represent a discharge from the ground-water system. When the head in the aquifer becomes lower than the land surface opening of the spring, the spring dries up. The higher the head in the aquifer above the altitude of the spring opening, the more water discharges from the spring. Thus, springs are usually treated as nonlinear head-dependent discharge boundaries that have zero flow when the head in the aquifer becomes lower than the altitude of the spring, using the same mathematical representation as that used for a drain (fig. 3D).

Recharge at the Water Table

Recharge is a term used to describe many of the processes involved in the addition of water to the saturated zone (Wilson and Moore, 1998). This discussion will focus on recharge at the water table from sources other than surface-water bodies.

Recharge from precipitation is frequently an important source of water to ground-water systems. In many if not most locations, precipitation (rainfall or snowmelt) soaks into the ground and recharges the water table over the areal extent of the aquifer system. The amount of recharge is usually determined externally to the model and is calculated as the amount of precipitation minus surface runoff and evapotranspiration at land surface. The recharge rate is usually then incorporated into ground-water flow models as a specified-flow boundary condition along the top boundary of the ground-water model. Although this approach is very straightforward conceptually, several nuances must be considered when implementing the simulation of areal recharge in ground-water models.

One nuance is in selecting the best method to simulate recharge in three-dimensional ground-water models in which the top surface of the saturated system (the water table) extends into different model layers. The conceptual issue is whether the recharge should enter only the top layer or should enter the uppermost active layer. Usually, the recharge is input to the uppermost active layer. How recharge occurs in nature and how it is treated in any specific model must be carefully considered. The model MODFLOW provides options that allow different approaches for simulating recharge at the water table (McDonald and Harbaugh, 1988); some other models do not allow different conceptualizations and the way in which these models treat the input of recharge must be specifically considered to ensure accuracy.

Another nuance is not related to the physics of recharge, but rather to the numerical methods used in many ground-water models. In some unconfined ground-water systems with areal recharge, the saturated zone becomes thinner near the lateral boundaries of the system. In simulating these systems, models solving the nonlinear problem calculate the saturated thickness as part of that solution. Because it is a nonlinear problem in which the saturated thickness is a function of the head, the solution techniques must iterate to obtain a solution. In iterating towards a solution, the heads may ‘overshoot’ the correct head and cause a cell or areas of the model to become incorrectly represented as dry, which causes the model cell or cells to be cut out of the active model area and made inactive. Under this condition, the areal recharge that should be entering the system does not do so because the simulated lateral extent of the saturated system has been prematurely or incorrectly reduced. This causes the model to account for a reduced amount of recharge, which results in an incorrect water budget and usually a truncated model extent that would not exist in the actual system. The only way to detect this is to carefully evaluate the results of any simulation and evaluate the extent and the amount of recharge simulated.

If the model is not converging to the correct model extent and amount of recharge, then non-standard approaches must be employed to ensure that the boundary is reproducing the actual system. Some of the approaches that investigators have used include: (1) reformulation to allow for the re-wetting of dry cells, (2) modification to parameters used in the solution of the equations (the matrix solver), (3) a modified transient approach, and (4) better starting heads for the matrix solution. The re-wetting approach is one that allows for inactive ‘dry’ cells to become active depending on the heads in the surrounding cells (for example, McDonald and others, 1992). The re-wetting approach, however, is also subject to numerical difficulties, and is not always a solution to the problem. The approach of modifying solver parameters is one whereby an attempt is made to slow down the convergence of the matrix problem in order to approach the correct solution smoothly and not cause any cells to dry up prematurely. Specifics of this approach depend on the matrix solution technique used. The modified transient approach is one in which a steady-state solution is obtained by simulating the problem as a transient condition and calculating the heads through time until they no longer change. This transient approach slows down the rate of convergence so that the correct solution is reached gradually through time. In steady-state problems, the use of starting heads that are close to the final solution can also remedy the problem. Some investigators have used fixed saturated thicknesses to simulate the problem and obtain an approximate solution; then, this approximate resultant head solution is used as starting heads for the nonlinear water-table problem. With this technique, the equation solver tends to oscillate less and approach the solution smoothly without making cells dry up incorrectly, because the starting heads are closer to the actual nonlinear solution. These approaches do not always work, however, and the investigator is responsible to ensure that the solution is reasonable.

As an example of the discussion above, consider a one-dimensional water-table system with a sloping impermeable bottom that contains a specified head and extends 5,000 meters, with an areal recharge rate of 0.5 m/yr. The starting head for the equation solution is specified at 20 meters, which is above all the bottom elevations of the cells but yet close to the magnitude of the expected results. Figure 5A is a cross-sectional view of a finite-difference representation of the steady-state solution. The cell farthest from the specified head is simulated as being dry. The total recharge flowing to the specified head cell for a 500-meter width is 2,740 m^3/d. The convergence criterion of the model was met and the mass balance was perfect. Now consider figure 5B, which is the result of a simulation of the same problem, except the starting head for the matrix solution was set at 100 meters. As is shown in figure 5 and table 2, three cells are now simulated as being dry. The result is that less recharge is simulated as entering the model and the heads and water budgets are reduced accordingly, with only 2,055 m^3/d being represented as recharge entering the system for a 500-meter width. Although both solutions converged and had perfect mass balances, at least one of them is incorrect. Because it is a nonlinear problem, it is not easy to determine which is the correct solution. The rate of convergence and the method of making cells inactive must be considered and evaluated. After evaluating these aspects, it seems that the first model is most likely correct. In the second model, the iterative solution, in attempting to converge, apparently overshot the bottom of some of the cells, which prematurely or erroneously truncated the area from the active model domain, and resulted in the wrong problem being solved. The model developer or user must carefully evaluate nonlinear problems and monitor the rate of convergence to ensure that cells that should be part of the active problem domain are not removed.

Recharge in valley-fill ground-water systems, particularly in arid areas, commonly originates from runoff from surrounding mountains or higher elevation locations (fig. 6). This runoff can be conceptualized as being either diffuse or channeled. Diffuse runoff conceptualizes the process of surface runoff as occurring all along the boundary edge of the modeled ground-water system and the recharge is usually simulated as a specified-flow boundary along the top layer of the model. Channeled runoff conceptualizes the surface runoff as occurring in stream channels and the resultant ground-

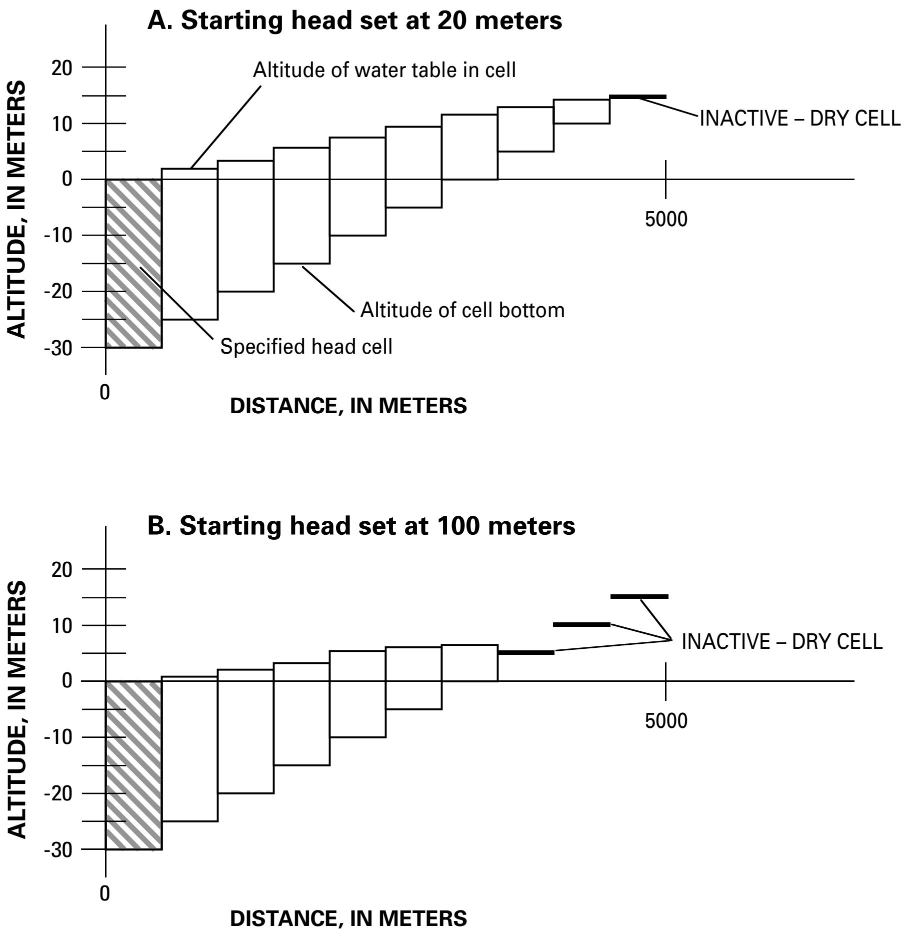


Figure 5. Cross-sectional view of a finite-difference representation simulating a variable thickness ground-water system with flow to a specified head due to areal recharge: (A) starting head set at 20 meters, and (B) starting head set at 100 meters.

water recharge is usually simulated by means of a subset of the methods used to simulate streams, that is, either as a specified-flow condition or by a nonlinear method such as streamflow routing (Prudic, 1989). A potential additional source of recharge in valley systems is ground-water flow from the surrounding mountains. If the rocks of the mountains do contribute flow, that flow must be estimated and usually is conceptualized as a specified flow entering the valley-fill ground-water system along the boundary.

Earth Materials of Low Hydraulic Conductivity

No earth material is completely impervious to water. Many earth materials, however, have very low hydraulic conductivities and thus contribute relatively small amounts of water to adjacent permeable ground-water systems. Depending upon the conceptualization of the system and the objectives of the study, a boundary between a permeable ground-water system with appreciable flow and a surrounding body of earth material of low-hydraulic conductivity that contributes a negligible amount of water commonly is treated as a no-flow boundary. This is a specified-flow boundary (table 1) across which the flow is exactly zero. For example, in the hypothetical valley-fill aquifer system shown in figure 6, if the bedrock contributes an insignificant amount of water to the valley-fill deposits, the boundary of the valley-fill deposits could be conceptualized as an impermeable or ‘no-flow’ boundary. This no-flow boundary is approximate because some flow probably enters the actual system across this boundary. The objectives of the study and the relative magnitudes of the flow in the bounding material, as compared to the flow in the aquifer material, are key to assessing the assumption of negligible flow that can be approximated as no flow. In some systems, assuming a no-flow boundary may be reasonable for flow-system analysis, but such an assumption may not be appropriate for transport analysis in which the actual path of a particle is important.

Inter-Basin Flow

Many alluvial ground-water systems underlie major river systems. These ground-water systems form sub-basins along the entire length of the river, for example, the alluvial basins along the Rio Grande in New Mexico (Wilkins, 1998), as shown in figure 7. In an attempt to simulate flow in one of the sub-basins, the boundary that controls the exchange of ground water between adjacent basins can be important and difficult to represent. As always, the key to a successful simulation effort is to select the boundary of the model to coincide with a feature in the actual system that can be simulated reasonably well and that will minimize the effect of any artificial approximation. This location is usually where the basin narrows near the stream and is reasonably far from the area to be stressed. Depending upon the situation, the boundary can be represented as a no-flow, specified-flow, specified-head, or head-dependent flow boundary. None of the choices are perfect because the actual ground-water system does not begin or end at the boundary location, but is continuous along the stream. Thus, any boundary condition to be used in a numerical ground-water flow model involves trade offs that must be carefully evaluated on a case-by-case basis and monitored during the use of the model.

Table 2. Heads calculated for the same hypothetical ground-water flow system with areal recharge and two different initial heads.

Node number	Head calculated with the initial head at 20. m	Head calculated with the initial head at 100. m
1	0.00	0.00
2	1.93	1.46
3	3.83	2.86
4	5.68	4.17
5	7.49	5.38
6	9.24	6.42
7	10.90	7.20
8	12.45	Dry
9	13.81	Dry
10	Dry	Dry

Ground-Water Evapotranspiration

Ground-water evapotranspiration is the process by which water is removed from the saturated ground-water system by plant usage (transpiration) or evaporation. This is not to be confused with evapotranspiration at land surface or in the unsaturated zone. Most ground-water models take into account the rate of evapotranspiration at land surface and the unsaturated zone by subtracting it from the rate of precipitation in the calculation of a net recharge rate. How and where in the saturated ground-water system evapotranspiration occurs should be thoroughly conceptualized to ensure that only the loss from the saturated zone is considered.

Some investigators have inadvertently ‘double counted’ ground-water evapotranspiration by both removing it from the calculated areal recharge rate and simulating it in the model, causing the system to be incorrectly represented. An example of ‘double counting’ and incorrectly applying

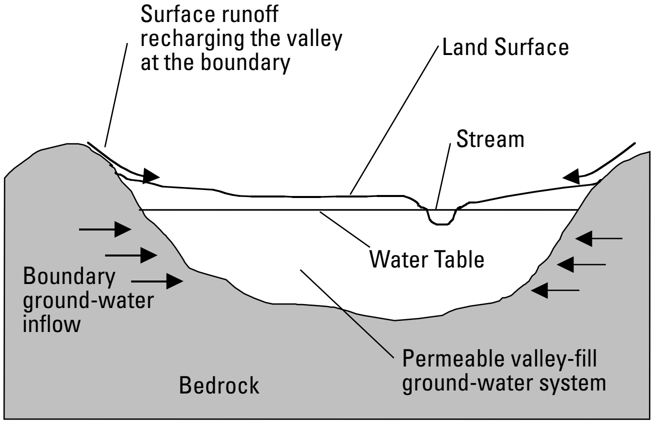


Figure 6. Diagram of a valley-fill aquifer system that is recharged by infiltration of surface runoff and lateral ground-water inflow from the surrounding bedrock.

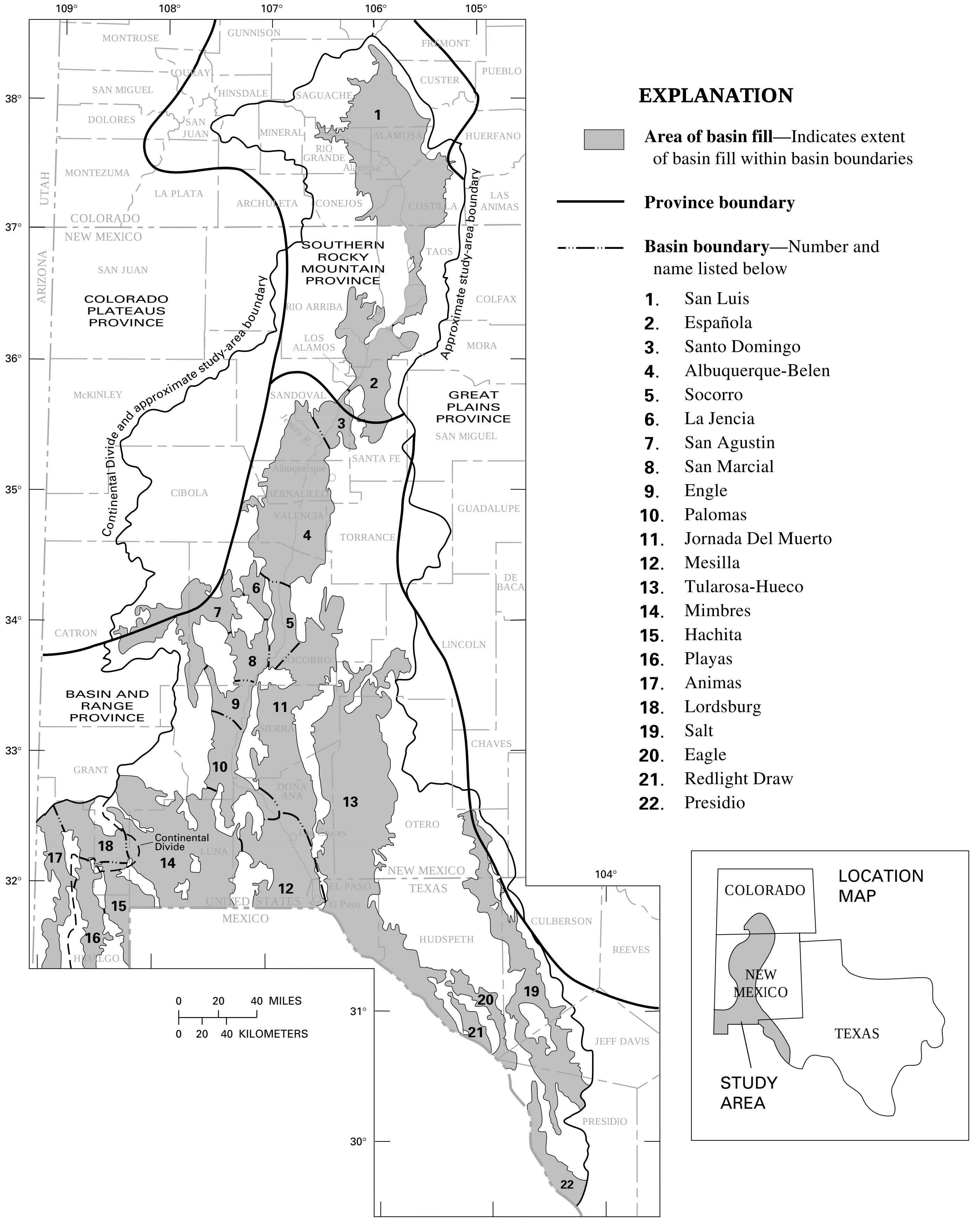


Figure 7. Location of the alluvial basins studied by the Southwestern Alluvial Basins Regional Aquifer-Systems Analysis. The basins along the Rio Grande form a continuous stretch of alluvial deposits. (Modified from Wilkins, 1998)

ground-water evapotranspiration is in cases in which the areal recharge rate is calculated by means of hydrograph separation and ground-water evapotranspiration is included in the simulations. Investigators use hydrograph separation to determine the base flow of a stream, which represents the outflow from the ground-water system. Some investigators have then equated the outflow of the system (the base flow) to the recharge under unstressed conditions. The base flow, however, actually represents the areal recharge minus the water removed by ground-water evapotranspiration. Thus, the ground-water evapotranspiration has already been taken into account in the estimate of areal recharge and should not also be simulated in the numerical model. Conversely, if the location of the evapotranspiration is important and should be simulated in the model, then any estimate of recharge must not be based solely on the estimates of base flow. The physical processes to be simulated must be carefully evaluated to ensure that evapotranspiration is represented appropriately.

Ground-water evapotranspiration is usually conceptualized as occurring at a rate that varies with depth. It is assumed that the nearer the water table is to the land surface, the greater the likelihood that plant roots will be in direct contact with the water table and the greater will be the amount of water withdrawn from the saturated zone. In MODFLOW, evapotranspiration is approximated as a linearly varying rate that ranges from a maximum at elevations at or above land surface and decreases to zero below some depth, referred to as an extinction depth (fig. 8). Because evapotranspiration loss from the saturated zone cannot be measured directly, the various conceptualizations are difficult to check independently. Most investigators realize that methods of accounting for ground-water evapotranspiration in numerical models are usually a crude approximation of what actually occurs in nature. Because of the inability to compare simulated evapotranspiration losses with measured losses, investigators must rely on conceptualizations that are internally consistent and reasonable, although less than perfect.

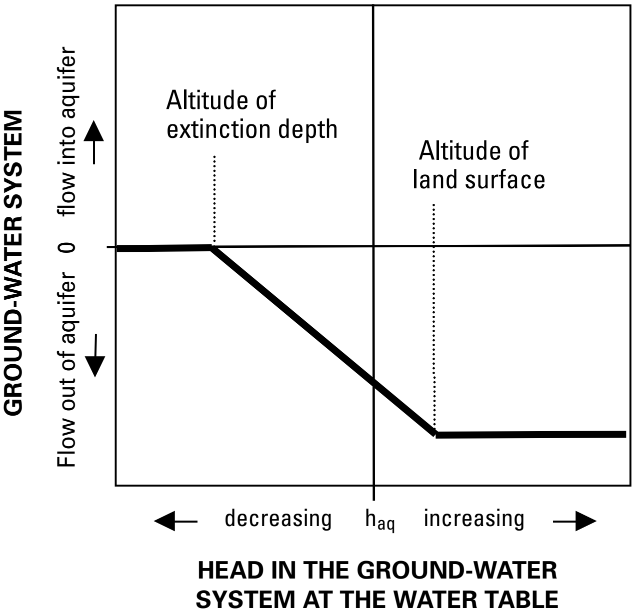


Figure 8. Graph showing the simplified mathematical relation between the head in the aquifer and outflow from the aquifer due to evapotranspiration as used in the ground-water flow model, MODFLOW.

Spatial Changes in Density of Water

The density of the water moving through the ground-water system is important in calculations of the fluid's mass balance and its velocity. Numerical models that are designed to simulate ground-water flow usually assume a constant density for water and solve a mass balance equation with head as the dependent variable. The amount of total dissolved solids in the water and the temperature of the water affect the density of the water. To accurately account for the effects of density on a flow system, a variable density flow and transport model is required, because the flow is dependent on the density distribution. There are, however, simplified approaches to account for density variations in models that are constructed primarily to simulate the movement of the fresh water in an environment that contains fresh water and denser salt water (Reilly, 1993).

In systems in which the density changes abruptly between a fresh water zone (or volume) and a more dense 'salty' zone, the boundary between the fresh water and the salt water can be conceptualized and approximated as a no-flow interface (fig. 9). The fresh water tends to flow along and on top of the salty water and negligible flow crosses the interface under equilibrium conditions. The interface can be approximated as a zero specified flow (no flow) if the density between the two fluids changes abruptly. The position of the boundary is dictated by the magnitude of the fresh-water head [see Reilly (1993) for a more detailed explanation]. In constant-density models, the location of the boundary can be calculated only under steady-state conditions or cases in which the movement of the boundary is assumed to be of negligible importance to the problem. In dual-density models, where both the fresh-water zone and the salt-water zone are simulated as two distinct systems, each with their own constant density [for example, the SHARP model by Essaid (1990)], the no-flow boundary between the two systems can move transiently because the movement and storativity of fluids in both systems are taken into account.

In layered coastal systems, such as that shown in figure 9, the physical processes that occur in the confining unit must also be conceptualized and the appropriate boundary condition selected. Depending upon the hydraulic conductivity, pressure, and density distributions, this boundary between the fresh water and salt water at the confining unit can be conceptualized as either a no-flow boundary or a head-dependent flow or 'leaky' boundary (Essaid, 1990; Reilly, 1990). Conceivably, water can flow along the fresh water – salt water interface in the lower aquifer (fig. 9) and discharge across the confining unit into the salty ground water overlying the confining unit. In this conceptualization, the confining unit would contain fresh water, the rate of discharge of

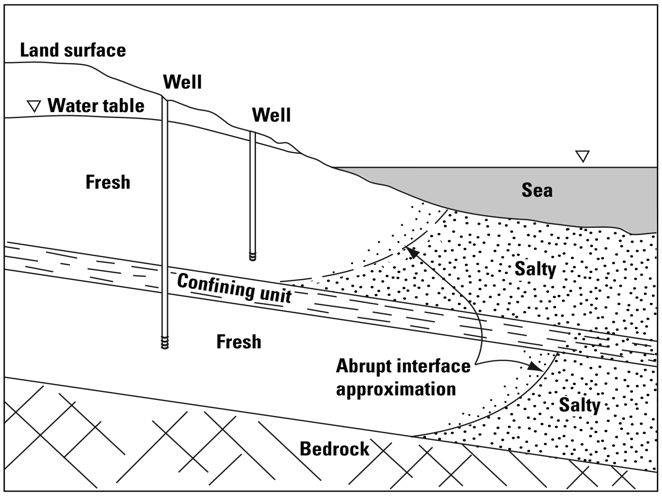


Figure 9. A ground-water system containing fresh and salty water in a coastal environment (Modified from Reilly and Goodman, 1985).

that fresh water into the overlying permeable zone of salty ground water would be small, and the fresh-water discharge would not change the density of the overlying salty water because it would mix thoroughly with the overlying water. In a fresh-water simulation, the specified head at the head-dependent boundary would be the equivalent fresh-water head at the top of the confining unit, and the dependent head would be at the bottom of the confining unit and would be calculated as part of the model solution. The confining unit is conceptualized as containing fresh water, and the calculation of leakage, as illustrated in figure 4, would be a valid estimate, even in this two-density system. Obviously, this approach is an approximation, but it does mimic some of the coastal systems observed in nature.

Ground-Water Divides

A ground-water divide is not really a boundary in nature. A ground-water divide is defined in the Glossary of Hydrology (Wilson and Moore, 1998) as: (a) a ridge in the water table or other potentiometric surface from which the ground water represented by that surface moves away in both directions, and (b) the boundary between adjacent ground-water basins. Figure 10 shows a ground-water divide in an unconfined aquifer for natural undisturbed conditions (fig. 10A) and under stressed conditions (fig. 10B). Ground water on each side of the divide moves away from the divide and no flow crosses the divide. When a system is pumped (stressed), the location of the divide can move in response to this pumping. Although a divide is a ridge in the head distribution or the boundary between adjacent ground-water basins, the ground-water system is continuous across the divide, and, therefore, the divide does not physically bound the system.

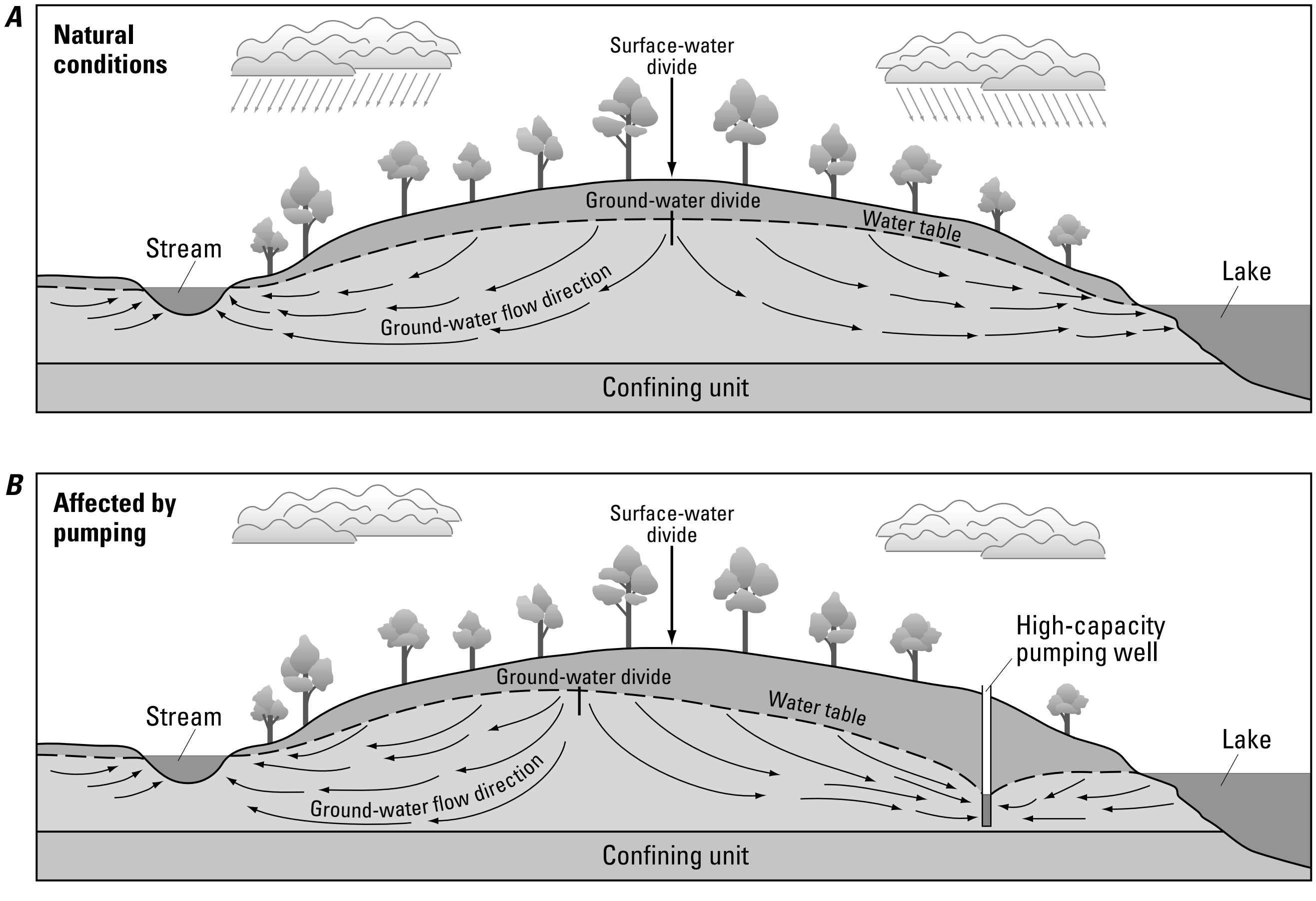


Figure 10. Diagrams showing generalized ground-water flow (A) under natural undisturbed conditions and (B) affected by pumping (From Grannemann and others, 2000).

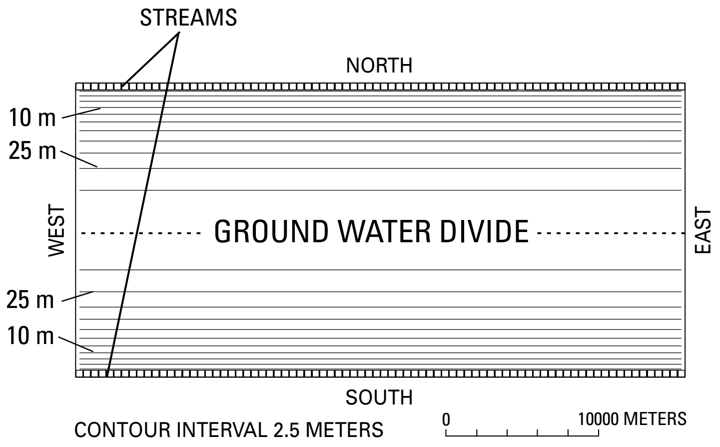


Figure 11. Head distribution for a hypothetical ground-water system consisting of two streams separated by a ground-water divide.

Ground-water divides are frequently simulated as no-flow boundaries in ground-water flow models to limit the areal extent of the system being analyzed. Depending upon the objectives of the study, this may or may not be appropriate. The effect of simulating a ground-water system as being bounded by a ground-water divide can be subtle but yet very important to some of the possible simulation results. The following example illustrates some of the inherent difficulties in using a ground-water divide as a boundary in a ground-water flow model.

Figure 11 shows a ground-water system that is 40 km long and 20 km wide. A stream with a head of 0 meters bounds each edge (north and south edges) of the rectangular system and there is a no-flow boundary along the east and west edges. The hydraulic conductivity is a uniform 50 m/d and an areal recharge rate of 0.5 m/yr (0.00137 m/d) occurs over the entire system except for the cells that contain the streams. The bottom of the system is an impermeable base at an elevation of –30 meters, so that under unstressed conditions, the saturated thickness of the system varies from a minimum of 30 meters at the streams to a maximum of 59.2 meters at the divide. Because of the symmetry of the system, a ground-water divide forms midway between the two streams. The flow to each stream is 520,600 m^3/d, and the head at the divide is 29.2 m.

When one half of the natural undisturbed system is simulated and the divide is represented as a no-flow boundary, the resultant flows and head distribution are identical to that for half of the original system. In both the full-system and the half-system simulations, the maximum head at the divide is 29.2 m and the flow to the stream is 520,600 m^3/d. If the system is stressed, however, the two representations of the system produce different results. The key to whether the difference is important depends upon the objectives of the study using the model.

To illustrate the differences that can occur in the two different system representations (the full system and the half system that uses the ground-water divide as a no-flow boundary), their response to one discharging well is determined. A well located halfway between the ground-water divide and the northern stream is simulated with a discharge rate of 2,447 m^3/d. The resultant head distributions for the full system and half system representations are virtually identical, as shown in figure 12. The ground-water divide in the full system has moved in response to the pumping, but the movement is very small when the system as a whole is considered. The simulated drawdown in the cell containing the well is 0.66 m in the full system and 0.71m in the half system when the ground-water divide is a no-flow boundary.

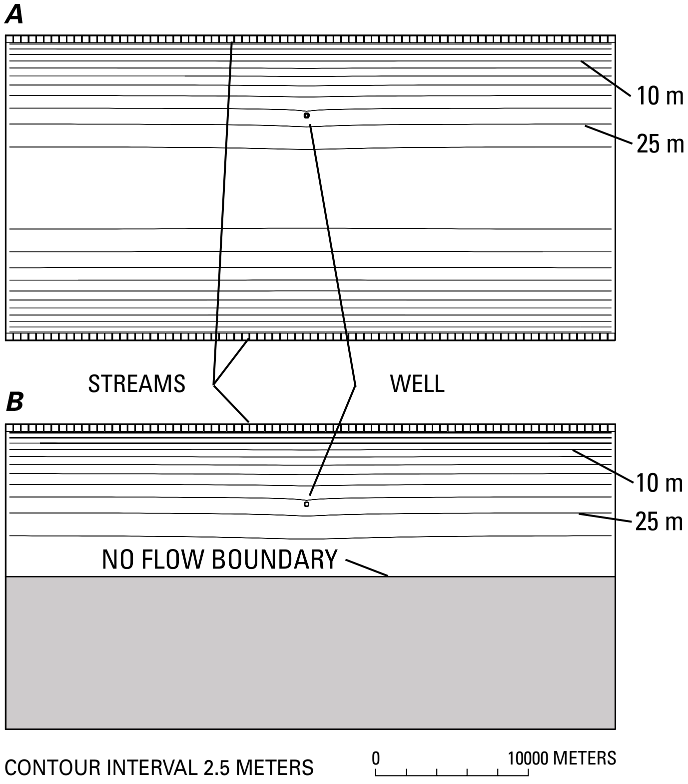


Figure 12. Head distribution: (A) for the full hypothetical ground-water system consisting of two streams separated by a ground-water divide, and (B) for a similar ground-water system in which a no-flow boundary is simulated at the initial ground-water divide, resulting in half of the original system being used to simulate the system. In both systems, one well is discharging at a rate of 2,447 m^3/d.

Examination of the simulated water budgets in the two systems, however, provides a different perspective. In the full-system simulation, the river closest to the well decreased its flow by 1,818 m^3/d and the river on the opposite side of the divide decreased its flow by 628 m^3/d, which accounts for the total pumpage. In the half system with the ground-water divide simulated as a no-flow boundary, all the water pumped comes from the only stream simulated and equals 2,447 m^3/d. Thus, the simulated water budgets for the two different conceptualizations are substantially different.

In the full system, the ground-water divide moves in response to pumping. The amount of areal recharge that flows to the stream on the opposite side of the divide from the well is decreased. Although the movement of the divide is subtle, it can account for a substantial redistribution of flow. In the half system, however, where the divide is represented as a no-flow boundary, this redistribution cannot take place and some error is introduced. The amount of error depends in part on the distance of the well from the stream, or conversely, the proximity of the well to the divide. Determining when it is appropriate to represent the divide as a stationary no-flow boundary can be problematic.

In summary, the representation of a ground-water divide as a no-flow boundary in a model of an unstressed system is conceptually consistent with its role in nature. When the ground-water system is stressed, however, the representation of a ground-water divide as a no-flow boundary, without taking into account its potential for movement, may introduce significant error. Thus, as always, the objectives of the study and of the model must be consistent with the decision to use a ground-water divide as a boundary in a model of the flow system or to extend the domain of the simulation to coincide with a boundary that is fixed in space.

Artificial Boundaries that are Not Physical Features

Ground water exists continuously under the land surface. Identifying the domain of a ground-water system to be studied, therefore, always requires judgments as what to represent as the boundary of the system. In locations where very permeable material is adjacent to poorly permeable material, the definition of a bounding surface is usually straightforward. The selection of surface features as boundaries is also usually straightforward, although as shown in this report, their mathematical representation is not necessarily straightforward. When the permeable aquifer material extends for large distances, however, how and where to set the boundary of a ground-water model to represent part of the extensive system becomes difficult. An artificial boundary is commonly defined to limit the size of a model that is representing only part of an extensive, continuous, permeable ground-water system.

Artificial boundaries, by their very definition, cannot accurately represent the response of the actual ground-water system to stress. Therefore, they must be selected carefully and checked frequently throughout the modeling exercise to ensure that the flow and head at the boundary are responding in a manner consistent with the conceptual model that was used in their selection. If at all possible, it is best not to use artificial boundaries in a model of a ground-water system.

When designing or considering the specification of an artificial boundary in a model, the functioning of the actual system must be considered. In particular, the source of water to the part of the aquifer being investigated must be represented as accurately as possible in the selection of the appropriate boundary. Usually, no-flow boundaries are defined along ground-water flow lines, and specified-head, specified-flow, or head-dependent flow boundaries are defined for locations where flow lines are not coincident with the location of the boundary. A key aspect in the design and selection of an artificial boundary is that both its location and type should be selected so as to minimize its impact on the analysis of the system under study.

An artificial boundary is specified in one of the examples used in this report, namely the representation of a divide (which is a ground-water flow line or surface) as a no-flow boundary. All the caveats associated with and discussed previously for such a divide being represented as a boundary apply to any artificial boundary condition.

EXAMPLES OF THE CONCEPTUALIZATION OF BOUNDARY CONDITIONS FOR TWO GROUND-WATER MODELS

The previous section discussed individual boundaries in ground-water systems. The conceptualization and mathematical representation of these boundaries is key to producing accurate models of ground-water systems. To illustrate the importance of boundary representation and the different possible conceptualizations, the features and water budgets of two models of actual ground-water systems are summarized. These summaries emphasize that the boundaries must be simulated such that the quantities and locations of the sources and sinks of water are reasonable and are consistent with the investigator's conceptual understanding of the system. The original system of units used in each case study is used here, even though they are different from those used in the rest of this report, in order not to introduce any round-off errors and to show the level of approximation used in the investigator's estimates.

Conceptualization of the Albuquerque Basin, New Mexico, Ground-Water Flow System

Approximately forty percent (about 600,000 people) of the total population of New Mexico (as estimated in 1990) lives within the Albuquerque Basin, which includes the City of Albuquerque. The Albuquerque Basin (also known as the Middle Rio Grande Basin) is in central New Mexico, and the Rio Grande flows through it (fig. 13). The climate in the Albuquerque Basin varies with altitude, but most of the basin is considered to be semiarid (Thorn and others, 1993). Because of ground-water pumping, water levels in the city of Albuquerque have declined by more than 130 feet since pumping began (Thorn and others, 1993). A computer model of the ground-water flow system (Kernodle and others, 1995) was developed to aid in understanding and managing the water resources of the basin.

The permeable part of the Albuquerque Basin is composed primarily of basin-fill deposits of the Santa Fe Group. Bedrock of the surrounding mountains and other low-permeability deposits bound the basin. In the steady-state predevelopment simulation, the head distribution (fig. 14) indicates that, in general, the ground water, as conceptualized by the model developers, moves from the basin boundaries and the Rio Grande and discharges primarily as evapotranspiration in the area near the Rio Grande.

The hydraulic properties of the basin-fill deposits are important in the determination of water movement within the

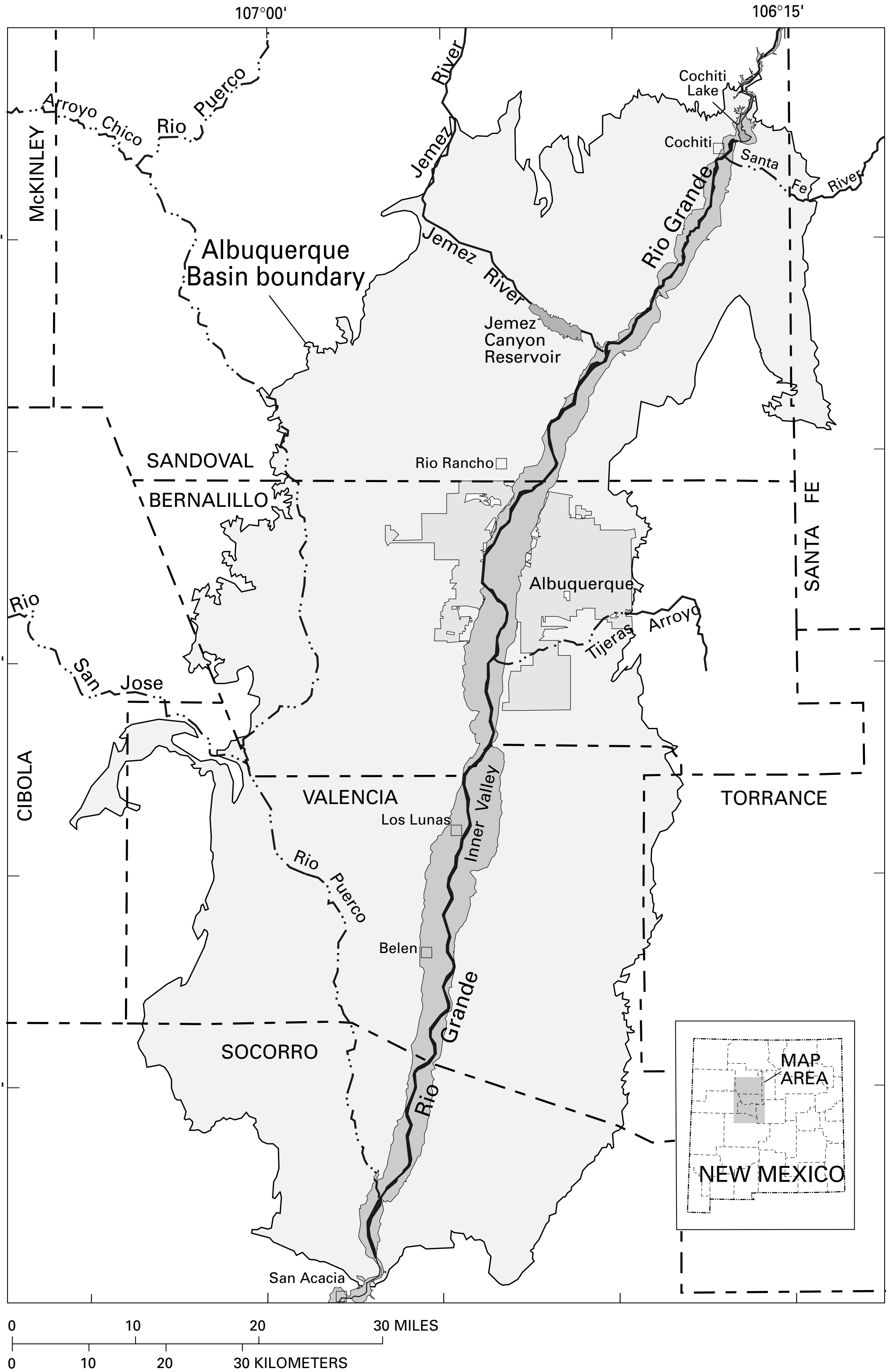


Figure 13. Location of the Albuquerque Basin, central New Mexico (Modified from Bartolino, 1999).

ground-water flow system, but the location and amounts of the sources and sinks of water to the system (that is, the boundary conditions) ultimately constrain the amount of water available for use. Therefore, accurate definition of the boundary conditions is very important to the accurate simulation of the basin. Kernodle and others (1995) used 11 layers and a finite difference grid of 244 rows and 178 columns to represent the Santa Fe Group aquifer with the computer code MODFLOW. The grid spacing varies from 656 feet (200 meters) on a side in the Albuquerque area to a maximum of 3,280 feet (1 kilometer) on a side at the basin margins. The investigators described in detail the physical boundaries of the basin and their representation of them in the model.

Major hydrologic boundaries caused by physical features of the ground-water flow system of the Albuquerque Basin are: (1) mountain front and tributary recharge, (2) ground-water inflow from adjacent basins, (3) irrigation seepage, (4) septic-field return flow, (5) river, canal, and reservoir leakage, (6) drain seepage, and (7) riparian and wetland evapotranspiration. The specific representation of the hydrologic boundaries as model boundary conditions is as follows.

Boundary conditions associated with physical features at the lateral extent of the model

The mountain front and tributary recharge was treated in the model as a specified flow boundary in the upper most layer of the model. The flow rates specified along the boundary and along the few major mountain front streams are shown in figure 15. This represents a major source of inflow to the ground-water system under predevelopment conditions. The ground-water inflow from adjacent basins was also treated as a specified flow condition, and these values are also shown on figure 15. However, the flow from adjacent basins was placed in model layers 5 through 9, rather than in the uppermost layer.

Boundary conditions associated with physical features at the bottom of the model

The bottom of the model was represented as a no-flow condition. There is no specific lithologic change at the bottom of the model, but rather the deposits decrease in permeability with depth. The vertical location of the boundary was selected such that the materials below the bottom of the model were thought to be of very low permeability and it was below the producing zones of any production wells.

Boundary conditions associated with physical features at the top of the model

The top of the model was represented as an unconfined aquifer. The water-table elevation (and therefore the saturated thickness) changes as part of the model solution. No areal recharge due directly to precipitation was simulated on the top boundary.

For seepage from excess irrigation water, it was assumed that approximately one third of the water applied to fields seeps through the soil profile and becomes recharge. After calculation, it was determined that this amount of recharge is one foot annually over the area being irrigated. Thus, a specified flow of one foot per year was simulated over the area of known irrigation. This area changed size and shape over the period of simulation and the area of the specified flow changed accordingly. The return flow from septic-field disposal was also treated as a specified flow. The population within each model cell, in areas not served by sewer systems, was assumed to discharge, to the uppermost active layer, 75 gallons per day per person, which is 75 percent of estimated rural per capita domestic use. The amount of flow changed over time on the basis of estimates of changes in population.

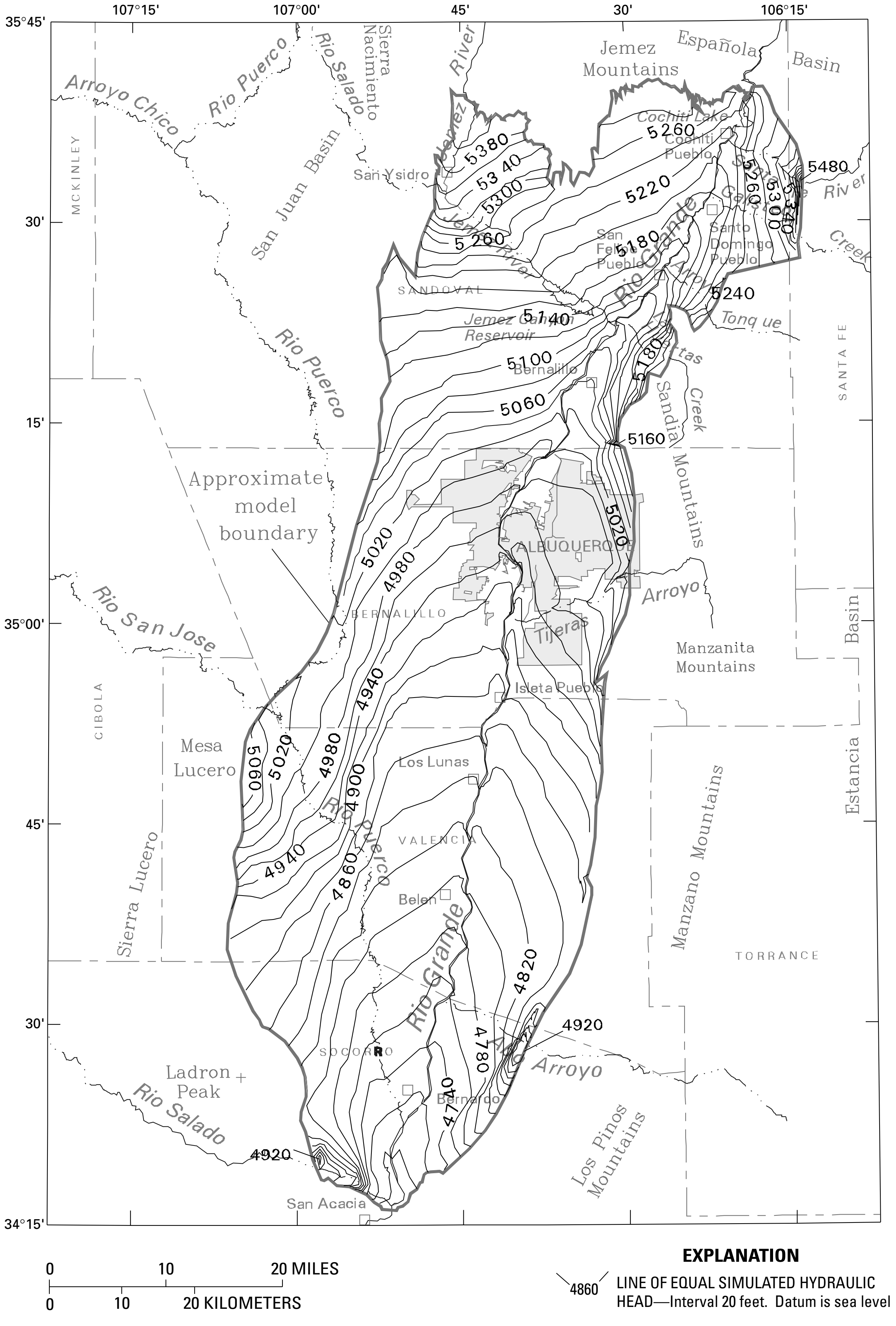
River, canal, and reservoir interaction is a key aspect of the Albuquerque Basin ground-water system. The MODFLOW 'River' package is used to treat these features as nonlinear, head-dependent flow boundaries (fig. 3E). The locations of the river, canals, and reservoirs changed through time after 1935, and these changes were simulated in the model. For the simulation period of 1901 through 1935 there were no canals and reservoirs, and only the Rio Grande was simulated.

A basin-wide network of drains was constructed in the Albuquerque Basin in the early 1930's. Riverside drains were constructed to intercept leakage from the Rio Grande that flowed toward areas in the valley that were at altitudes lower than the streambed. The 'Drain' package in MODFLOW was used to simulate these important hydrologic features as nonlinear, head dependent boundaries. Under this representation, the drain only gains seepage, and the rate is proportional to the altitude of the head in the aquifer above the drain elevation (fig. 3D). The drains, rivers, and canals can all exist in the same model cell, and although the local flow rates are not necessarily accurate, it is assumed that they produce the appropriate flows on a regional scale.

Riparian and wetland evapotranspiration was conceptualized as the major discharge boundary for the system under natural conditions. As discussed in the previous section, however, this component of a ground-water system is very difficult to measure and approximate mathematically. Land-use-cover data were used to approximate the extent of the area that would be undergoing evapotranspiration over time. The MODFLOW 'Evapotranspiration' package was used to simulate the process, with a maximum rate of 2.6 feet per year for heads at land surface, decreasing linearly to a rate of zero for heads at a depth of 20 feet or more below land surface. Because this major outflow from the ground-water system cannot be measured directly, it has to be checked for reasonableness against measured surface-water flows and other measurable components of the ground-water system.

Water budget for the system

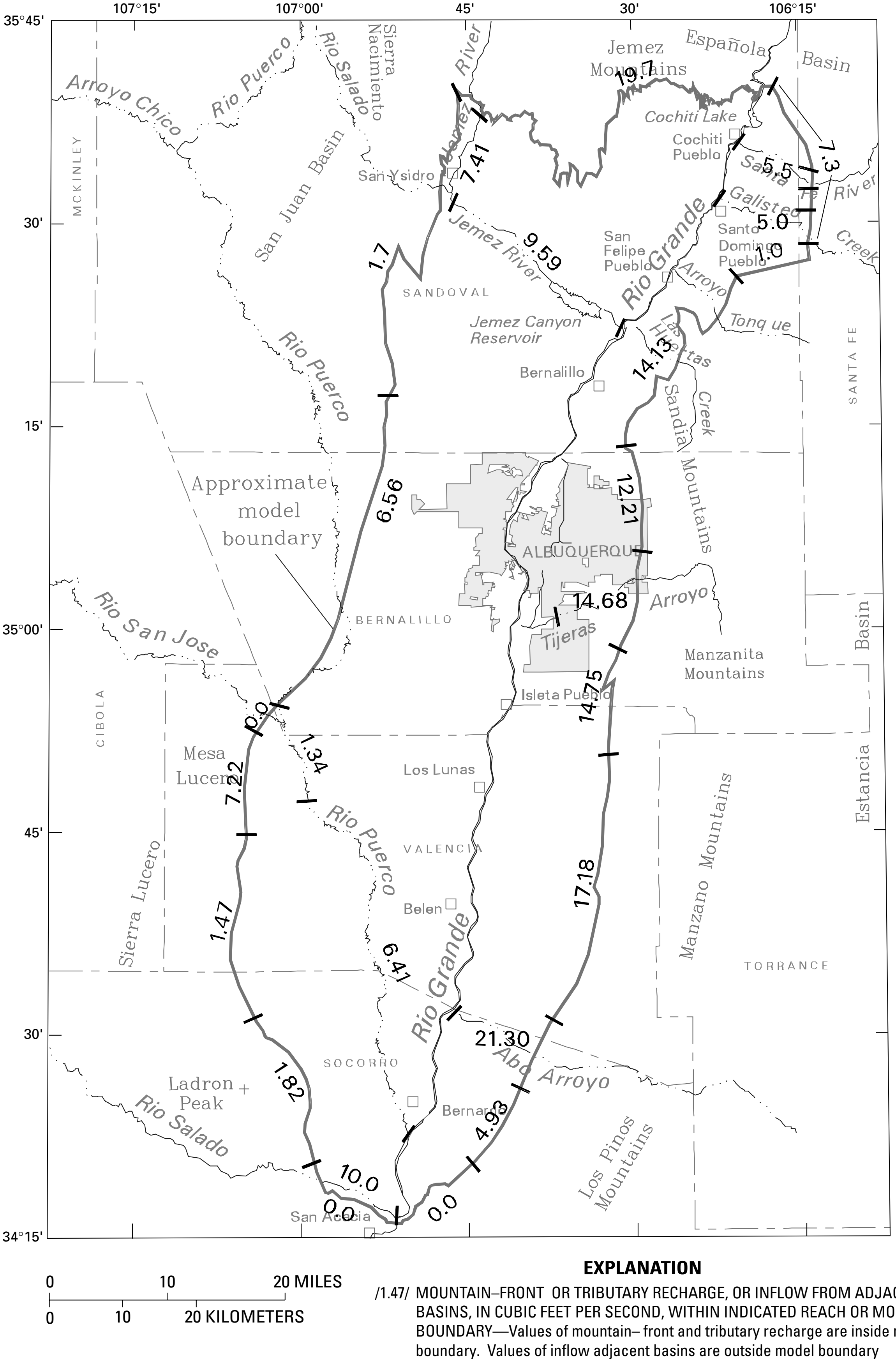
The simulated water budgets for predevelopment and for 1994, as presented by Kernodle and others (1995), are listed in table 3. The importance of the boundary conditions is readily observed in that all of the components in the table, except for water from storage and ground-water withdrawals, are from boundary flows. Only if the conceptualization and mathematical representations are appropriate does the simu-



EXPLANATION

4860 LINE OF EQUAL SIMULATED HYDRAULIC HEAD—Interval 20 feet. Datum is sea level

Figure 14. Simulated steady-state head in model layer 1 of the Albuquerque Basin model (Modified from Kernodle and others, 1995).



EXPLANATION

/1.47/ MOUNTAIN–FRONT OR TRIBUTARY RECHARGE, OR INFLOW FROM ADJACENT BASINS, IN CUBIC FEET PER SECOND, WITHIN INDICATED REACH OR MODEL BOUNDARY—Values of mountain– front and tributary recharge are inside model boundary. Values of inflow adjacent basins are outside model boundary

Figure 15. Estimated mountain-front and tributary recharge to the Albuquerque Basin, and inflow from adjacent basins. (Modified from Kernodle and others, 1995)

Table 3. Simulated annual water budgets for the Albuquerque Basin for predevelopment and 1994 (Modified from Kernodle and others, 1995). [All values are in acre-feet per year]

Mechanism	Predevelopment			1994		
	Inflow	Outflow	Net (inflow minus outflow)	Inflow	Outflow	Net (inflow minus outflow)
Mountain-front and tributary recharge	99,100	0	99,100	131,000	0	131,000
Ground-water inflow from adjacent basins	28,400	0	28,400	28,400	0	28,400
River, canal, and reservoir leakage	141,000	8,170	133,000	247,000	44,400	203,000
Drain seepage	0	0	0	0	219,000	-219,000
Riparian and wetland evapotranspiration	0	261,000	-261,000	0	89,200	-89,200
Irrigation seepage	0	0	0	28,300	0	28,300
Ground-water withdrawal	0	0	0	0	171,000	-171,000
Septic-field return flow	0	0	0	8,220	0	8,220
Aquifer Storage	0	0	0	109,000	27,800	81,200
Total	268,000	269,000	-500	552,000	551,000	920
Percent discrepancy			0.2			0.2

lation have any chance of accurately representing the actual system.

Conceptualization of the Long Island, New York Ground-Water Flow System

Long Island is bounded on the north by Long Island Sound, on the east and south by the Atlantic Ocean, and on the west by New York Bay and the East River (fig. 16). Long Island is divided into four counties—Kings, Queens, Nassau, and Suffolk. The source of water supply for the two western counties, Kings and Queens, which are part of New York City, is primarily surface water reservoirs located north of the city. Ground water, however, is the only source of fresh water for the population of Nassau and Suffolk Counties, which is greater than 2.5 million people.

The ground-water system of Long Island consists of a layered sequence of aquifers and confining units, which dip gently to the south and east (fig. 17). The system is underlain by crystalline bedrock that is virtually impermeable. Overlying the bedrock are hydrogeologic units of Cretaceous age, which are in ascending order: the Lloyd aquifer, the Raritan confining unit, and the Magothy aquifer. Above these are deposits of Pleistocene age. The Gardiners Clay, an interglacial marine clay that separates the Magothy and the overlying glacial aquifer, is present along the south shore of Long Island and has an irregular extent. Glacial deposits consisting primarily of moraine and outwash overlie all of these units throughout the island. Several other hydrogeologic units of local extent are also present.

Precipitation that infiltrates and percolates to the water table is Long Island's only natural source of freshwater because the ground-water system is bounded on the bottom by relatively impermeable bedrock and on the sides by saline ground water or saline bays and the Atlantic Ocean. About one-half the precipitation becomes recharge to the ground-water system; the rest flows as surface runoff to streams or is lost through evapotranspiration. Most of the precipitation that reaches the uppermost unconfined aquifer moves laterally and discharges to streams and surrounding saltwater bodies; the remainder seeps downward to recharge the deeper aquifers. Water enters these deeper aquifers very slowly in areas where confining units are present, but enters freely where the confining units are absent. Water in the deeper aquifers also moves seaward and eventually seeps into overlying aquifers.

Long Island's ground water has been developed over the past three centuries. The present phase of ground-water development on the island began in the early 1950's with the introduction of large-scale sewer systems in the most heavily populated areas. The purpose of the sewers was to prevent domestic wastewater from entering the aquifer system, because contaminants from this source were being detected in deep public-supply wells. Even though the sewers protect the aquifers from further contamination, they also prevent the replenishment (recharge) that the wastewater had provided to the ground-water reservoir through the domestic wastewater-disposal systems. The wastewater is now diverted to sewage-

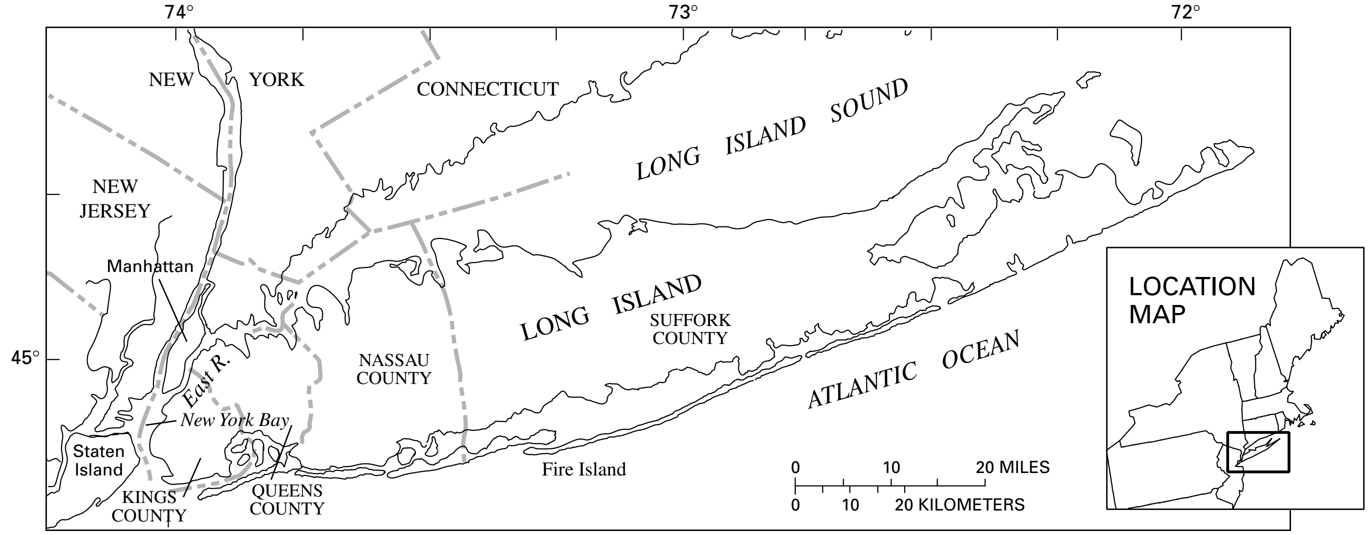


Figure 16. Location of Long Island, New York. (From Buxton and Smolensky, 1999)

treatment plants, whose effluent is discharged to the bays and oceans. The decrease in recharge has caused the water table in the sewered areas to be substantially lowered, the base flow of streams to be reduced or eliminated, and the length of perennial streams to be decreased. To aid in the management of this very important resource, several ground-water flow models have been developed (Getzen, 1977; Reilly and Harbaugh, 1980; and Buxton and Smolensky, 1999).

The latest ground-water flow model of Long Island (Buxton and Smolensky, 1999) is a three-dimensional finite-difference model that uses the MODFLOW computer program developed by McDonald and Harbaugh (1988). The

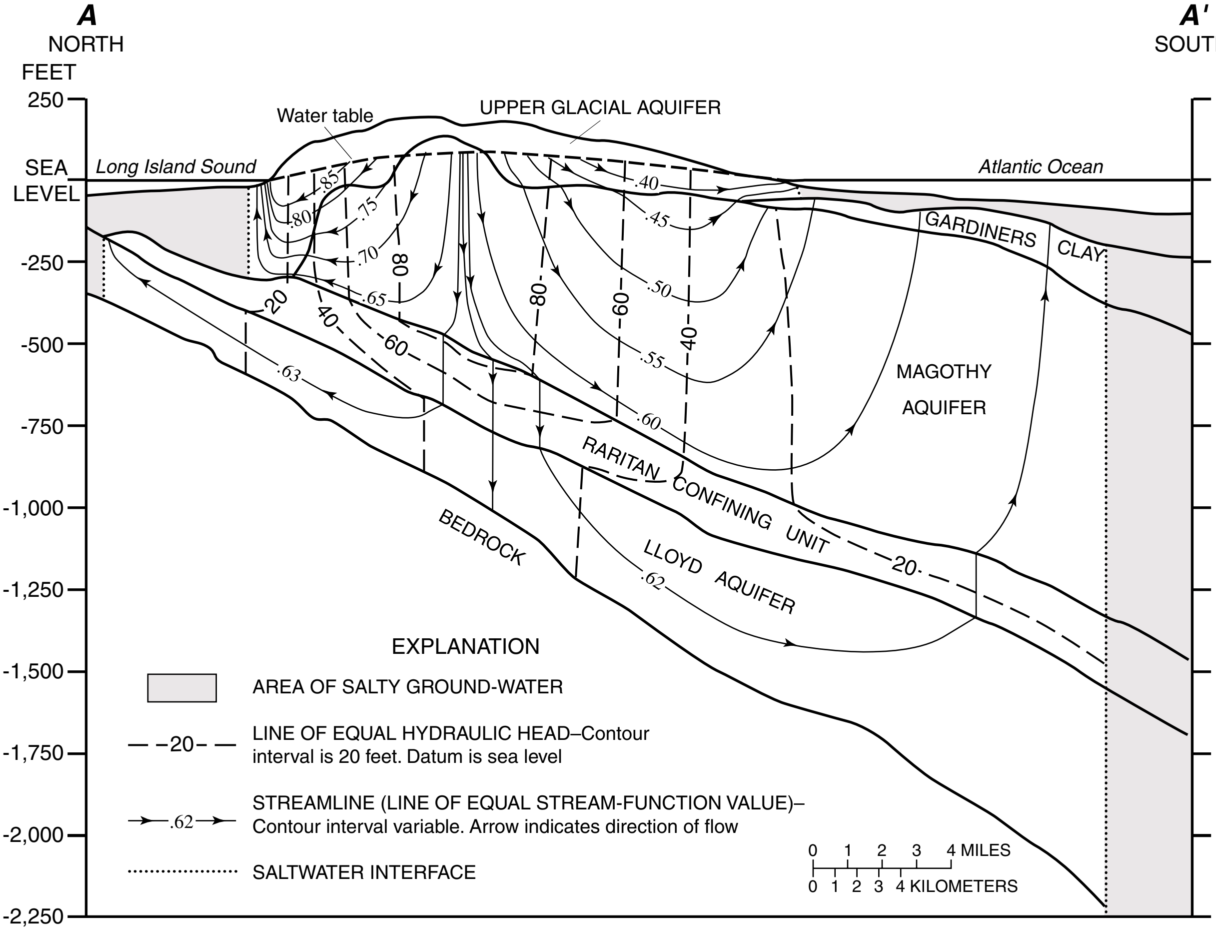


Figure 17. Hydrogeologic section of Long Island, New York. (From Buxton and Smolensky, 1999)

finite-difference grid has 46 rows and 118 columns (fig. 18), and each block is 4,000 by 4,000 feet. The model represents the aquifer units with 4 layers (fig. 19). The hydrologic features that form the boundaries of the Long Island groundwater system and their representation in the model are as follows.

Boundary Conditions Associated with Physical Features at the Lateral Extent of the Model

Salt surface-water bodies at the surface and salt-water interfaces at depth bound the lateral extent of the Long Island fresh ground-water system. The salt surface-water bodies (Long Island Sound, the Atlantic Ocean, Great South Bay, and others) are treated as a specified head in the top layer of the model. The saltwater interface is treated as a no-flow boundary in the deeper aquifers and model layers. In areas where the deeper aquifers are overlain by a confining unit and extend below a body of overlying salty ground water, subsea discharge can occur through the confining unit into the overlying aquifer that contains salty ground water. This subsea discharge boundary is represented as a specified head at the top of the confining unit, with the head at the top of the confining unit representing an equivalent freshwater head calculated to take into account the density difference between the overlying salty ground water and the discharging fresh ground water [see Buxton and Smolensky (1999) for an explanation of this specific boundary or Reilly (1993) for a general explanation of equivalent freshwater head].

Boundary Conditions Associated with Physical Features at the Bottom of the Model

The Long Island fresh ground-water system is bounded below by relatively impermeable Precambrian bedrock. Thus, the bottom boundary of the model representing the contact of the permeable deposits with the bedrock is simulated as a no-flow boundary.

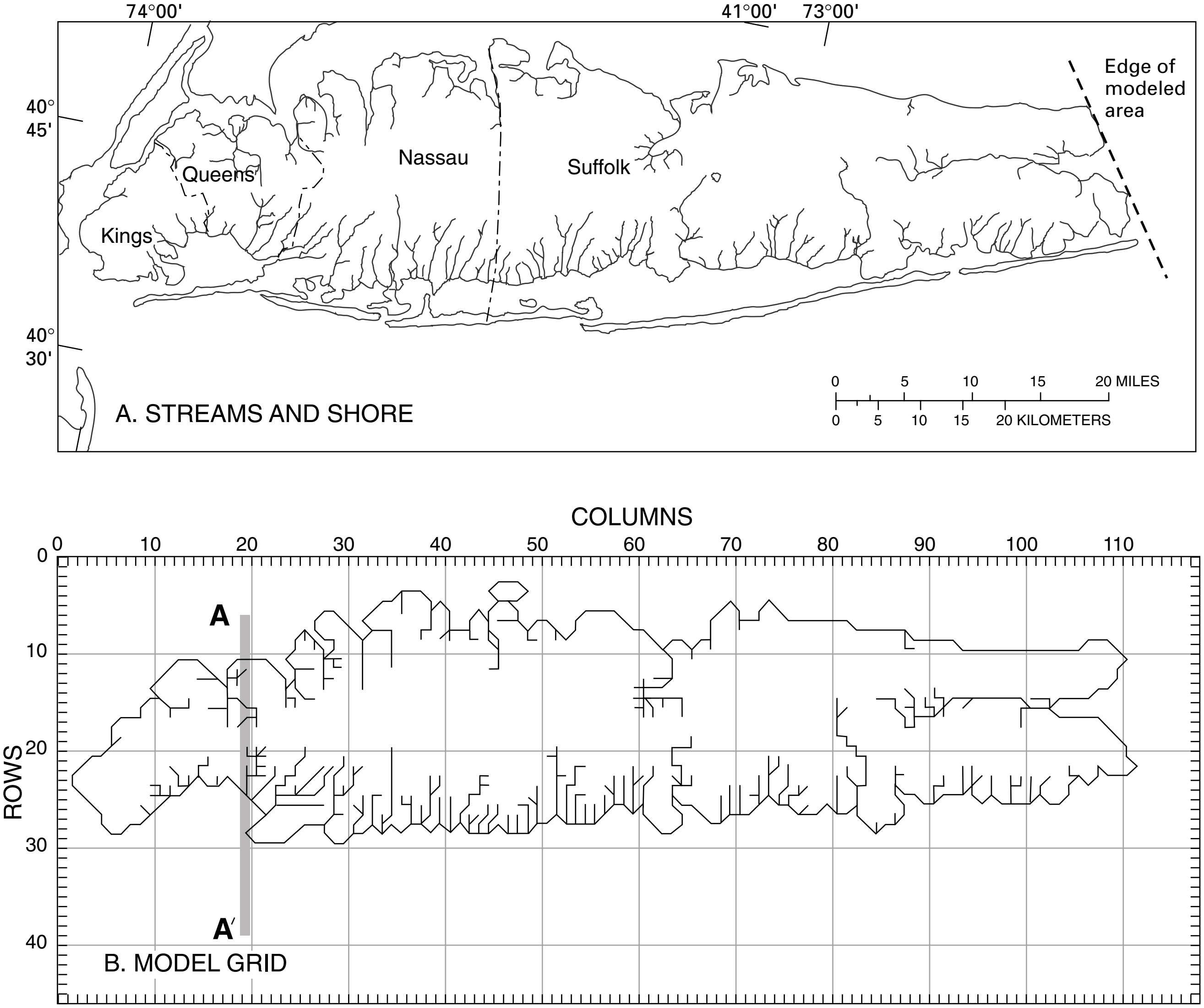


Figure 18. Areal representation of Long Island, New York, by the regional ground-water flow model: (A) Actual map view; and (B) Discretized map view. (Modified from Buxton and Smolensky, 1999)

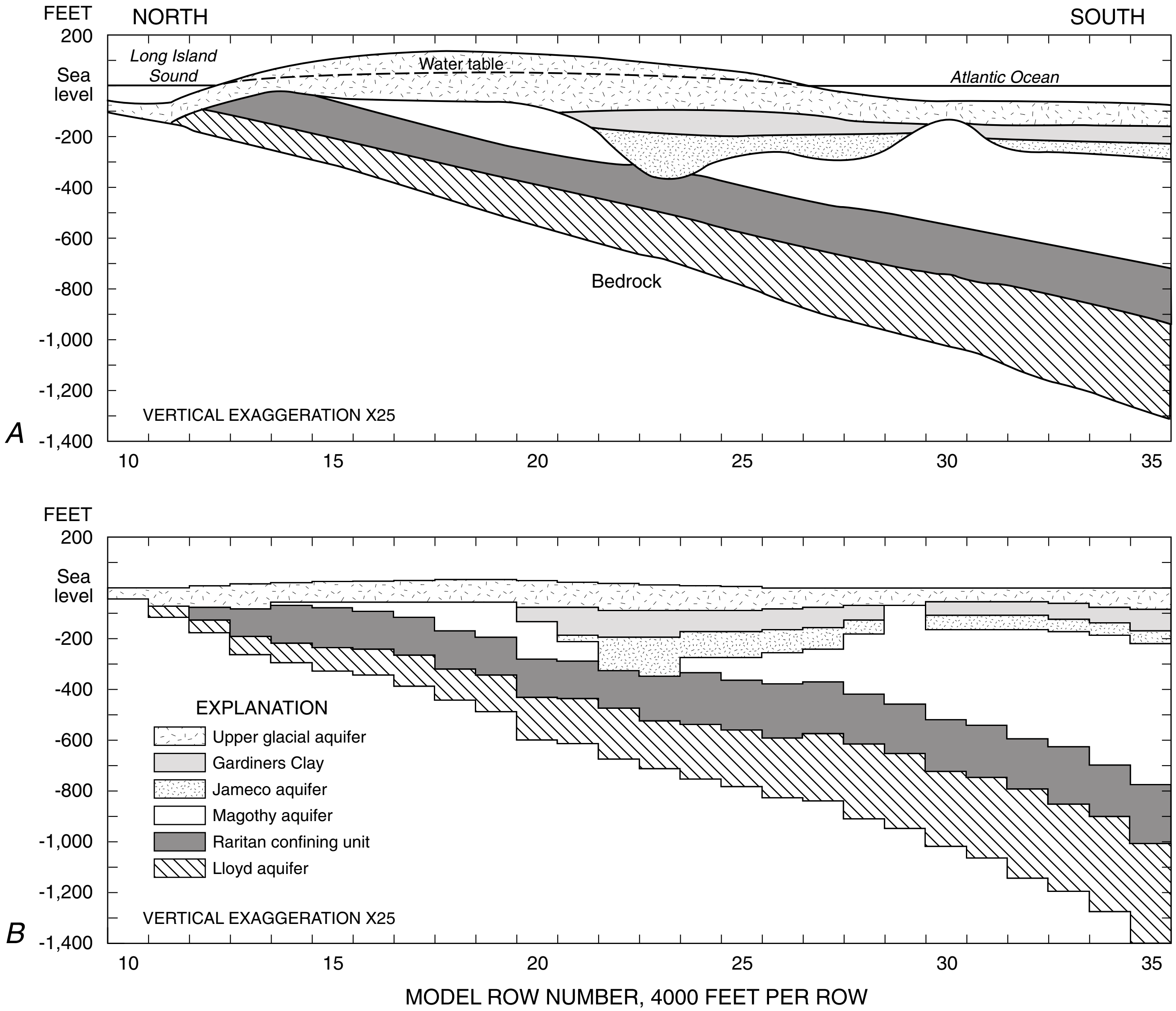


Figure 19. Cross-sectional representation of the ground-water flow system, Long Island, New York, in the regional ground-water flow model: (A) Actual cross section; and (B) Discretized cross section. Section located near A-A′ in figure 18 (From Buxton and others, 1999)

Boundary Conditions Associated with Physical Features at the Top of the Model

The top of Long Island's ground-water system is the water table that bounds the saturated ground-water system. The model represents the water table as a free surface that moves in response to stress. Areal recharge due to precipitation is simulated as a specified flow at the uppermost active cells.

Streams are represented in the model in two different ways, depending on whether the simulation is a steady-state simulation of known conditions or a transient simulation in which variations in ground-water discharge to the streams is to be determined. Streams are represented as specified discharge boundaries for steady-state simulations of known historical conditions, and as nonlinear, head-dependent strictly gaining boundaries (as a drain in MODFLOW) for simulations in which changes in base flow are simulated.

Water Budget for the System

The simulated water budgets for predevelopment and for the period 1968 to 1983, as presented by Buxton and Smolensky (1999), are listed in table 4. The importance of the boundary conditions is readily observed in that all of the components in the table, except for pumpage, are from boundary flows. Only if the conceptualization and mathematical representations of the boundaries are appropriate does the simulation have any chance of accurately representing the actual system.

Table 4. Simulated annual water budgets for the Long Island, New York ground-water system for predevelopment and the period of 1968-1983 (Modified from Buxton and Smolensky, 1999). [All values are in million gallons per day]

	Predevelopment			1968–1983		
Mechanism	Inflow	Outflow	Net (inflow minus outflow)	Inflow	Outflow	Net (inflow minus outflow)
Recharge from precipitation and returned water	1,126	0	1,126	1,293	0	1,293
Pumpage	0	0	0	0	407	-407
Stream discharge	0	460	-460	0	325	-325
Discharge at the shore	0	585	-585	0	503	-503
Deep subsea discharge	0	81	-81	0	58	-58
Total	1,126	1,126	0	1,293	1,293	0

SUMMARY AND CONCLUSIONS

When described mathematically, ground-water flow problems are classified as boundary value problems. This indicates that the selection of appropriate boundary conditions is critical to the accurate definition and analysis of the problem. In ground-water models, which are used for analyzing ground-water flow problems, the specification of the boundary conditions usually defines the source of water to the system and its ultimate manner of discharge. Thus, boundary conditions are one of the key aspects in the proper conceptualization of a ground-water system and representation of that system in a numerical computer model.

Conceptualizing the physical processes at the boundaries of a ground-water system and devising a mathematical counterpart that can be incorporated into a model is usually not straightforward. Appendix 1 lists many of the “Packages” that can be used in the U.S. Geological Survey Modular Three-Dimensional Ground-Water Flow Model (MODFLOW) to represent physical features of a ground-water system as mathematical boundary conditions. From this list, it is apparent that many different “Packages” can be used to simulate the same physical feature in a ground-water system. Depending upon the conceptualization and the expected use of the model, different mathematical representations can be used for the same feature.

The mathematical boundary conditions that represent physical features of the ground-water system being modeled are based on certain assumptions regarding the use of the model, the amount of stress that will be simulated, and the accuracy required. If the model is used to evaluate conditions that are no longer the same as the design assumptions, the simulation results will be invalid. The analyst must carefully evaluate the source of water to the ground-water system, the limits on the quantities of water available from the source, and potential changes to the system, and then select the appropriate mathematical counterpart. In addition, during the use of a model the analyst must continually check the simulation results to ensure that basic assumptions that were made regarding the boundary conditions during their selection are not violated.

Ground-water models are useful tools in analyzing ground-water flow problems. The proper design of a model, however, depends on a clear conceptualization of the flow system in nature and an understanding of the strengths and weaknesses of the various mathematical options available to simulate the various aspects of the actual system. A few of these mathematical representations of specific boundary conditions were discussed in this report to highlight the level of involvement that the analyst should have in the proper design and execution of ground-water models.

ACKNOWLEDGMENTS

The technical review and improvement of the report by Paul Barlow, William Cunningham, O. Lehn Franke, Arlen Harbaugh, and Douglas McAda is gratefully acknowledged. Chet Zenone provided editorial review and assistance, and Patricia Greene prepared the final report and illustrations.

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Appendix 1. List of "Packages" in the U.S. Geological Survey Modular Three-Dimensional Ground-Water Flow Model (MODFLOW) used to represent physical features of a ground-water system as mathematical boundary conditions

MODFLOW-PACKAGE NAME	PHYSICAL FEATURES THAT CAN BE SIMULATED	BOUNDARY-CONDITION TYPE	REFERENCE
Basic Package (BAS)	Stream, lake, ocean, wetland, interbasin flow, springs	Specified Head	McDonald and Harbaugh (1988)
Well Package (WEL)	Well, stream, interbasin flow, earth materials of low hydraulic conductivity	Specified Flow	McDonald and Harbaugh (1988)
Recharge Package (RCH)	Areal recharge or discharge	Specified Flow	McDonald and Harbaugh (1988)
General-Head Boundary Package (GHB)	Stream, lake, ocean, wetland, interbasin flow	Head-Dependent Flow	McDonald and Harbaugh (1988)
River Package (RIV)	Stream, lake, wetland	Nonlinear Head-Dependent Flow	McDonald and Harbaugh (1988)
Drain Package (DRN)	Stream, lake, drain, wetland, springs	Nonlinear Head-Dependent Flow	McDonald and Harbaugh (1988)
Evapotranspiration Package (EVT)	Evapotranspiration	Nonlinear Head-Dependent Flow	McDonald and Harbaugh (1988)
Block Centered Flow Package (BCF1)	Water table	Free-Surface	McDonald and Harbaugh (1988)
Stream Package (STR)	Stream, drain	Nonlinear Head-Dependent Flow	Prudic (1989)
Block Centered Flow Package 2 (BCF2)	Water table with rewetting	Free-Surface	McDonald and others (1992)
BRANCH Surface-Water Model Package (BRC)	Stream	Nonlinear Head-Dependent Flow	Swain and Wexler (1993)
Reservoir Package (RES)	Reservoir, lake, wetland	Nonlinear Head-Dependent Flow	Fenske and others (1996)
Flow and Head boundary Package (FHB)	Stream, lake, ocean, wetland, interbasin flow	Transient Specified Flow and Head	Leake and Lilly (1997)
Diffusion Analogy Surface-Water Flow Package (DAF)	Stream	Nonlinear Head-Dependent Flow	Jobson and Harbaugh (1999)
Lake Package (LAK3)	Lake, wetland	Nonlinear Head-Dependent Flow	Merritt and Konikow (2000)

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