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The discussion on the potential use of digital computer groundwater models was prepared for the Albuquerque District, Corps of Engineers, Albuquerque, New Mexico, as part of a water supply study of the Albuquerque Greater Urban Area (AGUA). Although the material presented was developed for the Albuquerque area, the concepts are applicable to the understanding of groundwater modeling generally. The discussion included both quantity and quality models and reasons why an agency may wish to undertake a modeling effort. Available computer programs were cited and the probable advantages and disadvantages of specific programs were given. Costs for prior modeling efforts of groundwater systems in other localities were also included as a guide to probable cost when considering the use of a digital computer groundwater model.

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POTENTIAL USE OF DIGITAL COMPUTER GROUND WATER MODELS[1]

by

David L. Gundlach[2]

PREFACE

The following discussion on the potential use of digital computer ground water models was prepared for the Albuquerque District, Corps of Engineers, Albuquerque, New Mexico, as part of a water supply study of the Albuquerque Greater Urban Area (AGUA). Although the material presented herein was developed for the Albuquerque area, the concepts are applicable to the understanding of ground water modeling generally. The discussion includes both quantity and quality models and reasons why an agency may wish to undertake a modeling effort. Available computer programs are cited and the probable advantages and disadvantages of specific programs are given. Costs for prior modeling efforts of ground water systems in other localities are also included as a guide to probable costs when considering the use of a digital computer ground water model.

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[1] From the preliminary report, Albuquerque Greater Urban Area Water Supply Study, prepared by The Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, California, 1978.

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SECTION 7

POTENTIAL USE OF DIGITAL COMPUTER GROUND WATER MODELS

CONTENTS

SECTION 7

POTENTIAL USE OF DIGITAL COMPUTER GROUND WATER MODELS

Introduction

A model, in the general sense, is a representation which attempts to explain the behavior of some aspect of the prototype system. It is always less complex than the real system it represents, and largely because of the complex interdisciplinary interests in ground water, models differ markedly in purpose, information requirements, assumptions, usefulness, and in the mathematical schemes incorporated.

The use of models to aid in the analysis of ground water systems has increased significantly in recent years (Konikow, 1970; Holcomb Research Institute, 1977). Many investigators find models useful including the applied researcher interested in verifying theoretical relationships, the hydrologist interested in developing the capability to predict effects of stresses (such as pumpage) on an aquifer system, and planners interested in the economic impact of the development of ground water resources.

Interdisciplinary modeling efforts are concerned with the quantitative description of the hydrogeologic properties and boundaries of aquifer systems, and with the response of aquifers to development and management practices. The models are tools used to evaluate ground water resources and to forecast the consequences of the utilization of aquifers. (Proper planning for the development of ground water resources requires testing of all possible schemes of development and appraisal of the relative merits of various alternatives). The modeling efforts are also concerned with the economic consequences of ground water development, with the practical sustained yields of wells and aquifers and with the interrelation between surface water and ground water.

Objectives. The objective of this section is to point out potential uses of ground water computer models in the management of the water resource of the AGUA. This includes models for both quantity and quality. Various reasons are cited as to when and why an agency or agencies should undertake a digital computer modeling effort and the different computer programs which might be applicable to AGUA are discussed and the probable advantages of each are given. Costs of the different modeling efforts are determined on the basis of similar studies done in other areas.

Digital Computer Models

In the early 1950's reservoir engineers looked to numerical methods adapted for digital computers to solve large scale flow problems. Early numerical reservoir simulations were severely limited by the size and speed of the digital computers of the period. By the late 1960's digital computers could compete with the electric analog for the solution of transient flow problems involving a few thousand nodes (computation points) in two space dimensions. With today's digital computers and powerful numerical techniques, three-dimensional problems involving up to 20,000 nodes can be solved.

Due largely to the widespread availability of the digital computer, numerical methods have replaced the electric analog in most applications. However, the electric analog model remains a very useful tool for problems involving multi-aquifer hydrologic systems which must be simulated with a large number of nodes.

With the development of high-speed computers, it has become feasible to develop numerical models that consider more realistic representations of complex hydrologic systems than was ever possible in the past.

Types of problems for which digital models have been or are being developed include, among others (Appel, et al., 1976):

(1) Flow in water-table aquifers in which relatively large changes in saturated thickness take place
(2) Flow in saturated or partially unsaturated materials
(3) Land subsidence resulting from ground water extraction
(4) Flow in coupled ground water/stream systems
(5) Coupling of rainfall-runoff basin models with soil moisture accounting and aquifer-flow models
(6) Interaction of economic and hydrologic considerations
(7) Predicting the transport of contaminants in an aquifer, and
(8) Estimating the effects of proposed development schemes for geothermal systems.

Many of these types of problems require that more than one equation be solved simultaneously. For example, general transport problems require the coupling and simultaneous solution of the partial differential equations that describe two (or more) components of a transient flow system. Typically, these would include, (1) an equation for pressure and (2) an equation for the concentration of each chemical constituent of interest.

A tabulation of the status of U.S. Geological Survey techniques in ground water modeling is shown in Table 7-1 (Appel, et al., 1976). If one contemplates an extensive modeling effort, then the documentation referred to in Table should be reviewed. The techniques consist of computer programs, analytical methods, and electric analog solutions which, with few exceptions, are applicable to transient conditions. In many cases more than one technique has been applied to similar ground water problems in order that the comparitive strengths of different methods can be evaluated and used to advantage. Such evaluations provide a rational basis for determining the method likely to be most efficient for particular types of problems. To state that a technique is in the verification phase means that tests are being made to see if model-derived solutions reasonably simulate observed responses. Techniques in the operational phase are being used to evaluate field problems.

TABLE 7-1.—*Status of ground-water modeling, U.S. Geological Survey*

	Phase of activity: Devel-op-men-tal	Phase of activity: Veri-fica-tion	Phase of activity: Op-era-tion-al	Phase of activity: Con-tinued im-prove-ment	Principal U.S. Geological Survey investigators	Recently published selected references
FLOW						
Saturated						
Two-dimensional						
Analytical	--	--	×	×	S. S. Papadopulos, R. L. Cooley.	Cooper (1966), Papadopulos (1967), Papadopulos (1966), Cooper and others (1965).
R-C Analog Networks	--	--	×	×	S. M. Longwill	Skibitzke (1960), Patten (1965), Stallman (1963b).
Numerical—Finite difference	--	--	×	×	P. O. Trescott	Trescott (1973), Pinder (1969), Maddock (1970).
Finite element—Galerkin	--	--	×	×	G. F. Pinder[1], R. L. Cooley	Pinder and Frind (1972), Frind and Pinder (1973).
Finite element—Variational	--	--	×	--	R. T. Hurr	Hurr (1972).
Three-dimensional						
R-C Analog Networks	--	--	×	×	S. M. Longwill	Skibitzke (1960), Stallman (1963a), Patten (1965).
Numerical (Finite difference)	--	--	×	×	P. C. Trescott	Trescott (1975), Bredehoeft and Pinder (1970).
Partly (or entirely) unsaturated						
One-dimensional						
Analytical[2]	--	--	×	--	C. D. Ripple, J. Rubin, T. E .A. Van Hylckama.	Ripple, Rubin, and Van Hylckama (1972), Stallman and Reed (1966).
Numerical—Finite difference	--	--	×	×	J. Rubin and C. D. Ripple	Rubin (1967, 1968a).
Finite element—Galerkin	--	×	--	--	----do	
Two-dimensional						
Numerical—Finite difference	--	--	×	×	----do	Rubin (1968b).
Cylindrical Region						
Numerical—Finite element—Galerkin	--	×	--	--	----do	Doherty (1972).
LAND SUBSIDENCE—Induced by ground water extraction						
Analytical	--	--	×	--	F. S. Riley	Riley (1969).
R-C Analog and Analytical	--	--	×	--	D. G. Jorgensen	Jorgensen (1975).
Numerical and Analytical	--	--	×	×	D. C. Helm	Helm (1974, 1975).
COUPLED GROUND WATER—*stream systems*						
Numerical—Finite difference	--	×	--	--	G. F. Pinder[1] and S. P. Sauer	Pinder and Sauer (1971).
Numerical and Analytical	--	--	×	--	A. F. Moench, V. B. Sauer, M. E. Jennings.	Moench, Sauer, and Jennings (1974); Luckey and Livingston (1975).
COUPLED GROUND WATER—RAINFALL-RUNOFF MODELS—Numerical	--	×	--	--	J. E. Reed and M. S. Bedinger and John Terry.	
COUPLED GROUND WATER—ECONOMIC SYSTEMS—						
Numerical	--	--	×	×	T. Maddock, III and J. D. Bredehoeft.	Bredehoeft and Young (1970), Young and Bredehoeft (1972), Maddock (1972, 1973, 1975).
COUPLED FLOW AND TRANSPORT OF CHEMICAL CONSTITUENTS						
Saturated system						
Conservative (or nonconservative trace constituents)						
Uniform density, inorganic						
Two-dimensional						

TABLE 7-1 (Cont'd)

Analytical	--	--	×	--	A. Ogata	Ogata (1976, 1970), Grove (1970).
Numerical—Characteristics	--	--	×	×	L. F. Konikow and J. D. Bredehoeft.	Konikow and Bredehoeft (1973), Robertson (1974), Bredehoeft and Pinder (1973).
Finite difference	--	×	--	--	D. B. Grove	
Finite element—Galerkin	--	--	×	×	D. B. Grove, J. Rubin, G. F. Pinder.	Pinder (1973).
Finite difference and finite element—Galerkin	--	×	--	--	D. B. Grove	
Variable Density						
Two-dimensional						
Analytical [2]	--	×	--	--	A. Ogata	Henry (1964).
Analog and Analytical [2]	--	--	×	--	G .D. Bennett	Bennett and others (1968).
Numerical—Characteristics	--	--	×	--	G. F. Pinder [1]	Pinder and Cooper (1970).
Finite difference [2]	--	×	--	--		Henry (1964).
Finite element—Galerkin	--	×	--	--	do	Segol, Pinder, and Gray (1975).
Three dimensional						
Numerical—Finite element—Galerkin	--	×	--	--	do	
Nonconservative, major constituents						
Uniform density						
Inorganic constituents (one-dimensional)—Numerical	--	×	--	--	D. B. Grove, W. W. Wood, J. Rubin, and R. V. James.	Rubin and James (1973).
Organic constituents (two-dimensional)—Numerical	×	--	--	--	J. B. Robertson and D. F. Goerlitz.	
Unsaturated						
Nonconservative, Major constituents						
Uniform density, inorganic constituents—Numerical	×	--	--	--	J. Rubin and R. V. James	
COUPLED FLOW AND TRANSPORT OF HEAT						
Single phase (hot water)						
Two dimensional						
Numerical—Finite difference	--	×	--	--	C. R. Faust and J. W. Mercer	Faust and Mercer (1976).
Integrated Finite difference	--	×	--	--	M. L. Sorey	Sorey (1975).
Finite element—Galerkin	--	×	--	--	J. W. Mercer and G. F. Pinder [1].	Mercer, Pinder ,and Donaldson (1975); Mercer and Pinder (1975).
Three dimensional						
Numerical—Finite element—Galerkin	×	--	--	--	G. F. Pinder [1]	
Two Phase (steam-water)						
Two-dimensional						
Numerical—Finite difference	--	×	--	--	C. R. Faust and J. W. Mercer	Faust and Mercer (1976).
Finite element—Galerkin	--	×	--	--	J. W. Mercer and C. R. Faust	Mercer and Faust (1975), Faust and Mercer (1975).
Three-dimensional						
Numerical—Finite element—Galerkin	×	--	--	--	G. F. Pinder [1]	
COUPLED FLOW AND TRANSPORT OF CONSERVATIVE (OR NONCONSERVATIVE TRACE) CONSTITUENTS AND HEAT (SINGLE PHASE)						
Two-dimensional						
Numerical—Finite difference [2,3]	--	×	--	--		Henry and Hilleke (1972).
Three-dimensional						
Numerical—Finite difference [3]	--	×	--	--	D. B. Grove, S. P. Larson	Intercomp (1976).

[1] Part-time investigator with USGS.
[2] Model limited to steady-state conditions.
[3] Model prepared for USGS under contract.

In many cases, investigators other than those given in Table 7-1 are, or have been, involved in the listed activity. The investigators listed can be contacted through the U.S. Geological Survey for information regarding the subject matter cited.

Digital Computer Models of the Ground Water Flow System

Digital computer modeling of an extensive flow system the size of the AGUA demands a highly organized approach to planning or management. It involves a relatively high initial cost and an intensive and coordinated data collection effort. However, it enables study of a much broader range of alternatives relating not only to flow but to quality and economic considerations.

Two-Dimensional Model of the Flow System. There are several well documented two-dimensional ground water computer programs available for simulating flow systems. Probably the one most commonly used is a two-dimensional finite difference model developed by Pinder (Pinder, 1970; Trescott, et al., 1976).

The two-dimensional formulation of flow in an aquifer system conceptualizes the physics of the process as being completely describable by movement in the horizontal directions, generally two orthogonal coordinate directions (flow in parallel horizontal planes being identical). The movement (velocity) of water in a given direction is in proportion to the negative gradient of the water table or piezometric surface and the permeability of the aquifer material. Continuity is preserved by requiring volume accounting through either changes in water surface elevations or changes in piezometric head and the compression and expansion of the water and of the porous framework of the aquifer. (The two-dimensional formulation does not specifically consider the vertical flow process and thus does not simulate well those systems with significant vertical components of flow and/or hydraulic conductivity). Solution to problems formulated in two space dimensions proceeds by discretizing the aquifer system into units, such as grids, and solving at successive time steps the relationships for flow movement at each designated computational point.

In order to get a feeling for what various terms mean it seems imperative at this point that a general description of the various aspects of a two-dimensional flow system be given. Since the ground water basin of AGUA is for the most part an unconfined, (except for localized areas exhibiting artesian characteristics), heterogeneous, anistropic aquifer, the following continuous form in two space dimensions is applicable:

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right) = S\frac{\partial h}{\partial t} + W \qquad (7\text{-}1)$$

where x, y are the orthogonal directions (L),

T_{xx} is the transmissivity in the x direction (L^2T^{-1}),

T_{yy} is the transmissivity in the y direction (L^2T^{-1}),

h is the hydraulic head (L),

S is the storage coefficient (dimensionless),

W is the net rate of recharge or discharge per unit area (LT^{-1}),

and t is time (T).

Equation 7-1 has been developed from the equation of continuity and Darcy's Law. In order to visualize the physical significance of this consider for the moment an idealized system as shown in Figure 7-1. The prism represents a small elemental volume taken through a compressible, horizontal, and confined aquifer of uniform thickness, b. Assuming that flow takes place in the x-direction only then inflow minus outflow represents the rate of change in storage. This can be written as

$$Q_1 - Q_2 = \frac{dV}{dt} \qquad (7\text{-}2)$$

where V is the volume of water contained in the elemental prism at a specific

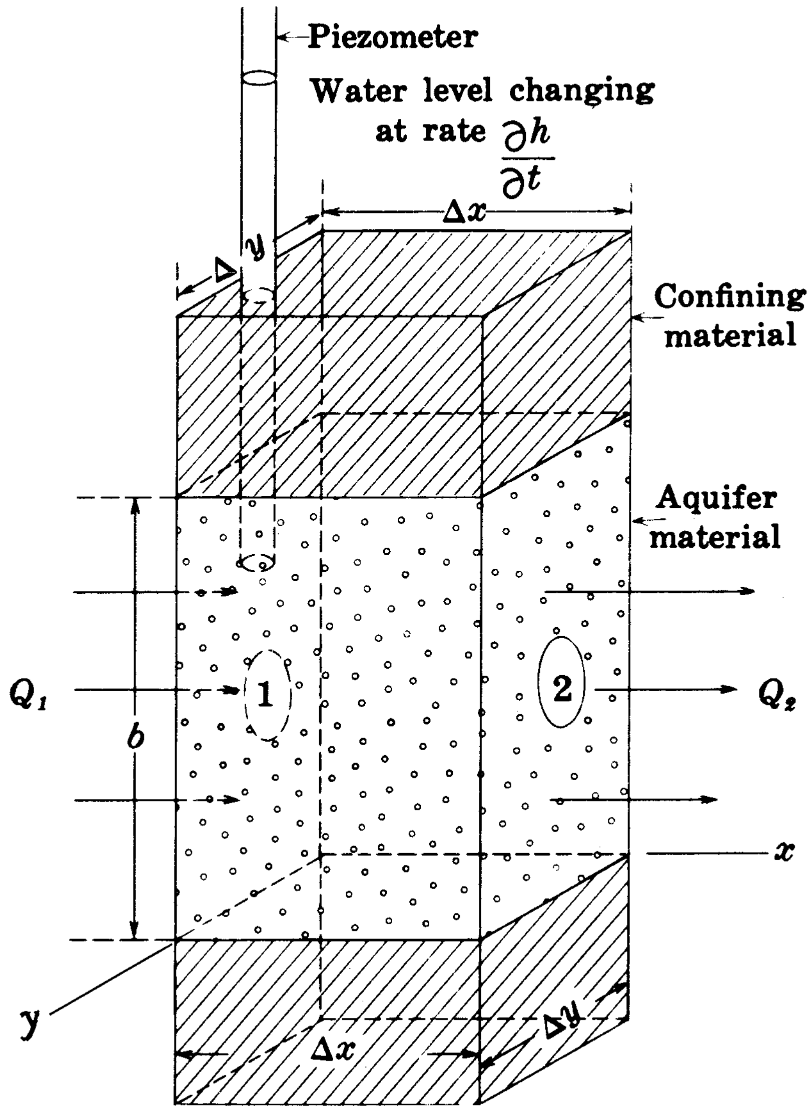


Figure 7-1

UNIDIRECTIONAL NONEQUILIBRIUM FLOW THROUGH AN ELEMENTAL PRISM OF A HORIZONTAL CONFINED AQUIFER.

(Bennett, G. D., Introduction to Ground-Water Hydraulics, U. S. Geological Survey, 1976) point in time. Since the storage coefficient, S, is the volume of water released from storage in a prism of unit area extending through the full thickness of the aquifer in response to a unit decline in head, Equation 7-2 can be rewritten as

$$Q_1 - Q_2 = S\Delta x\Delta y \frac{\partial h}{\partial t} \tag{7-3}$$

Assuming an isotropic and homogeneous aquifer and utilizing Darcy's Law, $Q_1 - Q_2$ can be approximated as shown below:

$$Q_1 - Q_2 \simeq Kb\Delta y\Delta x \frac{\partial^2 h}{\partial x^2} \tag{7-4}$$

The term Kb, represents the hydraulic conductivity of the aquifer times its thickness, and is called transmissivity or transmissibility, T. Now according to the equation of continuity, inflow minus outflow must equal the rate of change of water in storage within the prism of aquifer such that

$$T\Delta y\Delta x \frac{\partial^2 h}{\partial x^2} = S\Delta x\Delta y \frac{\partial h}{\partial t} \tag{7-5}$$

or

$$\frac{\partial^2 h}{\partial x^2} = \frac{S}{T}\frac{\partial h}{\partial t} \tag{7-6}$$

Equation 7-6 describes ground water movement under the simple conditions which were assumed; that is, where the aquifer is confined, horizontal, homogeneous, and isotropic, and the movement is in one direction. If horizontal components of motion normal to the x-axis were present, then inflow and outflow through the other two faces of the prism would have to be considered; that is, the two faces normal to the y-axis. In such a case

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S}{T}\frac{\partial h}{\partial t} \tag{7-7}$$

The relation given above is for two-dimensional ground water movement under the assumed consitions.

Although it is not important to understand the theory of partial differential equations, it is important to understand the flow process in relation to Figure 7-1. Later on in this section it will be shown how a two-dimensional grid is developed in conjunction with a ground model of the flow system and one should realize that each area of the grid system represents a prism of the type shown in Figure 7-1.

A more detailed analysis similar to the preceding methodology, for an unconfined, heterogeneous and anistropic aquifer results in the approximation, Equation 7-1. (It should be noted, however, that the calculation of the rate of change in storage for confined and unconfined systems involve completely different processes. Withdrawal from or addition to unconfined storage takes place at the water table whereas confined storage effects are distributed throughout the vertical thickness of an aquifer. Confined storage coefficient values usually range from 10^{-5} to 10^{-3} but unconfined values range typically from 0.01 to 0.35). An additional component, W, has been included to represent recharge to or discharge from the ground water body. Examples of this are: recharge due to precipitation, discharge due to pumpage, evapotranspiration, etc. Considering a prism, such as in Figure 1, but of such size as to include a well, then the term W would represent the rate of withdrawal from the prism due to pumpage.

As with ordinary differential equations, there will be an infinite number of expressions which will satisfy a partial differential equation; the particular solution required for a given problem must satisfy, in addition, certain conditions peculiar to that problem. These additional conditions, termed boundary conditions, establish the starting points from which the changes in h are determined.

Formal mathematical solutions of Equation 7-1 are available only for a small minority of field problems, representing simple boundary conditions. In most cases, we are forced to seek approximate solutions, using methods other than direct formal solution. One such method is the simulation of the above differential equation by a finite-difference equation, which in turn can be solved algebraically or numerically. Another is the finite element method for solving partial differential equations (Appel, et al., 1976; Pinder, 1974). Although finite difference schemes are presently the more widely used and documented, there are distinct advantages to the finite element method as mentioned later in this section.

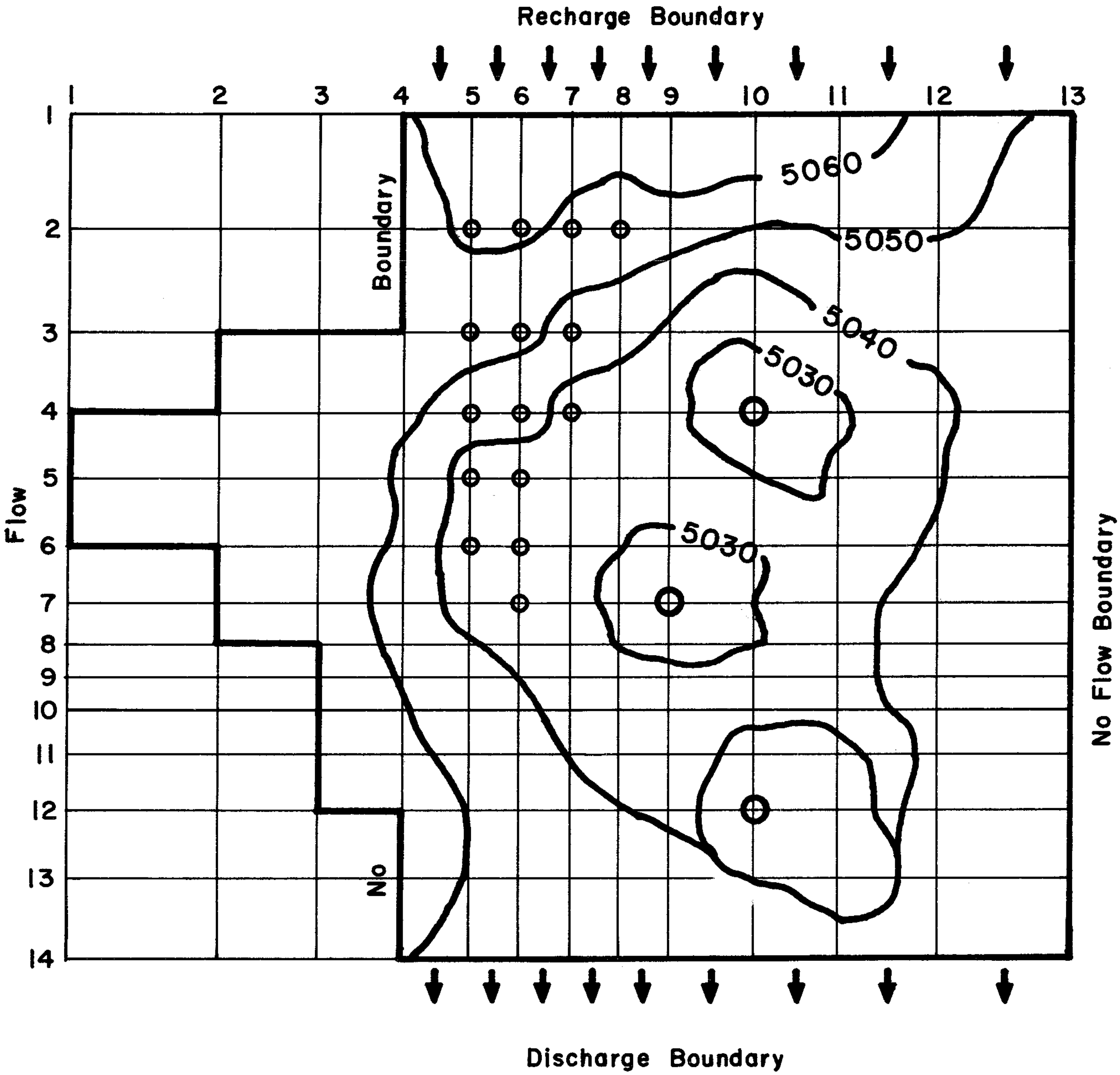
Where values of recharge or discharge, W, transmissivity, T, storage coefficient, S, are known for the AGUA aquifer system, then one can solve for the elevation of the water table. However, if values of T and h are known and a steady-state condition exists (where surface elevations of the water table remain essentially constant for some period of time), the time derivative of head equals zero, and the value of W can be found by using the remaining terms of the equation. Thus under steady-state conditions, $\frac{\partial h}{\partial t} = 0$, and

$$\frac{\partial}{\partial x} \left(T_{xx} \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y} \left(T_{yy} \frac{\partial h}{\partial y}\right) = W \qquad (7\text{-}8)$$

The preceding methodology is utilized in the computer program to compute elevations of the water table and/or estimate values of recharge and discharge throughout the aquifer system.

For the finite difference method, a two-dimensional grid network is superimposed on a plan view of the ground water reservoir as schematically shown in Figure 7-2. The intersection of any two lines on this grid is considered a node location and values of transmissivity, storage coefficient, and hydraulic head are input into the model at each node in the network. Boundary conditions and areas of recharge and discharge are also stipulated.

The two-dimensional computer programs available and utilizing the finite difference scheme, in general, will simulate ground water flow in a confined (artesian) aquifer, an unconfined (water-table) aquifer or a combination of the two. The aquifer may be heterogeneous and anistropic and have irregular



o Nodes representing recharge

O Nodes representing pumpage

—5060— Contours representing water table elevations

Figure 7-2. Two-Dimensional Variable Grid Network boundaries. The source term in the flow equation may include recharge from rivers to the aquifer, discharge from the aquifer to rivers, recharge from irrigation return and wastewater effluent, discharge due to evapotranspiration or pumping, recharge from a confined to an unconfined aquifer or discharge from an unconfined to a confined aquifer.

Considerations in designing the aquifer model for the AGUA, are listed below:

(1) Boundary conditions

The physical boundaries of the aquifer system should be included in the model if feasible irregardless of the project area (AGUA). It appears feasible that the eastern and western boundaries, as they are now delineated, can be incorporated in the model. The northern and southern boundaries of the aquifer are far removed from the project limits, such that they are impractical to include. Artificial boundaries could be designated at the most northern and southern limits of the study area if cost permits (cost is a function of the number of nodes). If the area of interest is in the immediate vicinity of the City of Albuquerque, the boundaries of the model could be located just far enough from the city as to have negligible effect on the computed water levels in that area during simulation. If the area of interest is the City of Albuquerque and all significant irrigated areas within AGUA the same criteria would apply. Where the northern and southern boundaries are located depends to a large degree on what the objectives of the model study are. Is one interested only in the impacts of pumpage on water table levels and Rio Grande flows, or the quality of domestic water now and at some later date, or the quality of subsurface water along the Rio Grande within AGUA? The cost of developing a two-dimensional model is dependent, of course, on the objectives of the model study.

In general boundaries are treated in the various computer programs as either constant head or constant flux (inflow or outflow). If the eastern and western boundaries of the AGUA are taken as the limits of the aquifer (impermeable boundaries), then the constant flux is zero. For the northern and southern boundaries, constant-head or finite-flux values would be specified.

(2) Initial conditions

In the AGUA the calibration of the model would probably begin from steady-state conditions or at that point in time where it is reasonable to assume the change in hydraulic head with time is essentially zero (see Equation 7-8). Since estimates of ground water levels (heads) are available for 1936 and since manmade stresses (pumpage, etc.) were relatively negligible at that time, a steady-state condition could be assumed for 1936. Steady-state conditions would permit estimates of recharge or discharge (such as evaporation, recharge from precipitation, recharge due to streams, etc.) at each node in the system.

(3) Finite-difference grid

A finite-difference grid, such as shown in Figure 7-2, can be variable within particular restraints.

Nodes representing pumping and observation wells should be close to their respective positions to facilitate calibration. If several pumping wells are close together, their discharge may be lumped and assigned to one node since discharge and head is distributed over the area of a rectangular grid. In the vicinity of the City of Albuquerque where wells in some cases are less than a mile apart, the grid space could be made finer, probably down to a mile or less depending on the area which will be modeled, in order to adequately simulate the stress due to pumpage on the system.

There are restrictions to the total number of nodes which can be economically and physically incorporated in a two-dimensional finite-difference model. Depending on the computer program and the computer facilities used for simulation, it could range from 10,000 to 20,000 nodes. If a variable grid spacing is incorporated (as would probably be the case for the AGUA), then there are restrictions also to the relative change in grid spacing which can be accommodated (the reader should check the documentation of various computer programs available). Nodes should also be placed close together where there are significant changes in transmissivity; and the axis of the grid oriented parallel to the principal direction of the transmissivity tensor (vector).

As mentioned previously, finite-element methods have been used to approximate the partial differential equations representing ground water flow (Pinder, 1974). This method utilizes irregular elements (triangles, rectangles which may be deformed in a specific way, etc.) instead of the rectangles common to the finite difference scheme. The rather arbitrary arrangement of nodes is a distinct advantage when modeling irregular boundaries and relatively localized areas of large stresses.

Calibration of a Two-Dimensional Model of the Flow System. The ultimate purpose of a model simulating the flow system is to predict changes in water levels in the aquifer caused by changes in stresses (pumpage, diversions, reservoir operations, etc.) on the system. Before a model can be used for prediction, it must be calibrated; that is water levels simulated by the stressed model must match measured water levels at any chosen time. In the AGUA this would mean that the ground water levels for 1936, 1960 and 1978, as determined in this study and prior studies (Bjorklund, et al., 1961; Reeder, et al., 1967; National Resources Committee, 1938), would be used in the calibration process.

In general the calibration process begins with the steady-state condition. (Although pumping wells existed in the AGUA in 1936, their impact on the ground water levels has been considered negligible). A map of transmissibility values and a ground water level contour map would be required for this particular point in time. Substituting map values of transmissivity, T, and hydraulic head, h, into equation 7-8, the computer program is used to compute recharge or discharge (net flux), W, at each nodal point in the system.

Plotting the proper sign (+ or -) of W, yields a map that indicates areas of recharge or discharge. Also the values of W can be compared, and any value of W that is considerably different from surrounding values is easily noticed. Values of W that are considerably different and obviously unreasonable can be adjusted by modifying T. The modified value of T is placed in the program and a computer run that computes a new value of W is made. This process is continued until a set of values for T, h and W is generated wherein the values for T and h do not yield values of W that are judged to be unreasonably large or small. Also, adjusted values of T or h are checked for consistency with adjacent values of T and h. (Values of h could be adjusted in this process if they were originally estimated in an area where very little or no observed data was available).

The next step in the model analysis generally involves determining differences in all recharge and discharge from the time of assumed steady-state conditions (1936) to 1960. These values are used to stress the model in discrete time steps so that the model will solve for h (for specified values of storage coefficient, S) in 1960, according to equation 7-1. The differences in recharge or discharge can only arise if there is a physical change that has occurred in the AGUA between 1936 and 1960 which affects the water resource. Examples of this would include new pumping wells, additional wastewater effluent, new irrigation canals and operations, changes in stream flow due to reservoir operation, etc.

A similar analysis would be required between 1960 and 1978 until model parameters satisfactorily reproduce the water-table levels for each of the designated years at each node in the system.

Data Required for a Two-Dimensional Model of the Flow System. In the AGUA the data that must be known or estimated for a two-dimensional ground water model of the flow system (whether finite-difference or finite-element) would include the following:

(1) A water-table level contour map for each of the years 1936, 1960 and 1978 for the area included in the ground water study.

(2) A map of transmissivity values for each of the years 1936, 1960, and 1975. (It could be that changes in saturated thickness due to progressive mining of the ground water body are insignificant when compared to the total saturated thickness. If this is the case throughout the aquifer system, then transmissivity values could be considered the same for each year without significant error).

(3) A map of storage coefficient values. At present this coefficient for the AGUA has been estimated as 0.20 but a more detailed analysis of this parameter is appropriate to calibrate the model. An average value of the storage coefficient can be obtained in the vicinity of a pumped well by measuring in one or more observation wells the decline of head with time under the influence of a constant pumping rate. Estimates can be made when there are no observation wells and only measurements of the drawdowns in the abstraction well are available. (Rushton, 1978) In a two-dimensional ground water model developed for the Modesto, California area the storage coefficient was estimated by using values of specific yield associated with the size and distribution of granular material (Page, 1977)

(4) Recharge from precipitation, wastewater and irrigation return.

(5) Pumpage and its distribution in time and space.

(6) Hydrologic parameters of any confining aquifer beds.

(7) Hydrologic parameters of river beds (particularly vertical hydraulic conductivity).

(8) Stages and flows in rivers and canals.

(9) Physical boundaries of aquifer system.

(10) Evapotranspiration rates from soils, agricultural crops, phreatophytes, etc.

The above data are placed at nodes in a particular grid system which is used for entering data in the flow equation. Additional data or better estimates of existing data would depend upon a sensitivity analysis (assuming that the model has been reasonably calibrated). A sensitivity analysis consists of determining model response when varying the magnitude of the model parameters by an amount proportional to the degree of uncertainty present in their determination. The degree of uncertainty can be determined statistically for some parameters and estimated for others.

Sensitivity testing consists of varying a given parameter in the model and recording the changes in simulated head as a result of the change in parameter. During a test, all other parameters are held at their adopted value. If model results are highly sensitive to a particular parameter, then a special effort should be made to determine that parameter as accurately as possible in order to improve the predicting accuracy of the model.

Three-Dimensional Model of the Flow System. With a three-dimensional model, the physics of the flow process is thought of as being completely describable by movement in three directions, generally three orthogonal coordinate directions. (In the two-dimensional system discussed previously, the flow process was described utilizing the x and y-coordinate directions as shown in Figure 7-1. For the three-dimensional simulation a vertical component is added). The equation of continuity now involves the determination of inflow and outflow through six faces of a prism instead of four as used in the two-dimensional analysis. The rate of change of water in storage is calculated in the same manner as previously described.

For the three-dimensional simulation, a grid network is superimposed on the area under study, and values of hydraulic conductivity, hydraulic head and specific storage are input to the model at each node in the network (see Figure 7-3). Boundary conditions, pumpage, recharge, etc. must also be included.

Vertical flow and variation in permeability with depth, for example, need no special consideration, thus giving the model added flexibility over a two-dimensional system.

Several finite-difference schemes for simulation of three-dimensional ground water flow systems have been documented (Trescott, 1976; Trescott, et al., 1976). The porous medium to be simulated may be heterogeneous and anistropic and have irregular boundaries. The uppermost hydrologic unit (aquifer system) may have a free surface. Stress on the system may be in the form of well discharge (or recharge), discharge due to evaporation, recharge from precipitation, etc. The model also permits the use of variable grid spacing.

Boundary conditions, initial conditions and the design of the finite-difference grid system are quite similar to that for the two-dimensional systems described previously. A disadvantage of a three-dimensional simulation is the size requirement (core) of the computer facility and the computation time involved. Both are proportional to the number of nodes representing the porous medium.

There have been successful applications of the three-dimensional ground water model to flow systems similar to AGUA, (U.S. Geological Survey, 1978) and several studies underway or proposed.

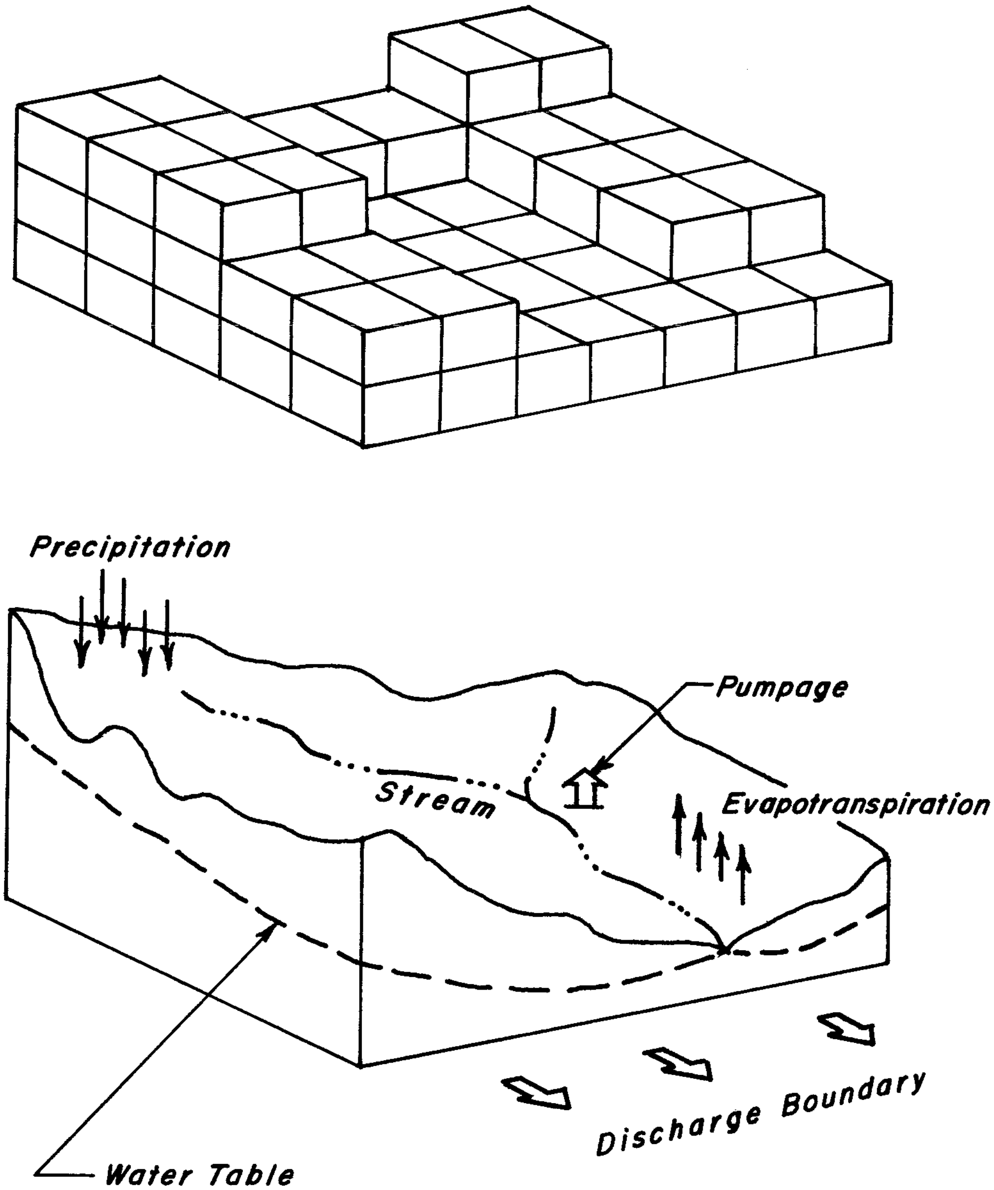


Figure 7-3. Three-Dimensional Grid Network

The calibration process and the data required are similar to that for the two-dimensional system. The added dimension though requires that storage and hydraulic conductivity be determined with respect to depth and that the directional aspects of hydraulic conductivity be thoroughly analyzed.

Digital Computer Modeling of Water Quality

The quality of water, because of its significance relative to various uses, has become of increasing importance. More intense efforts are now required to protect water resources from contamination and to predict the effects of man's activities on the chemical, physical and bacterial characteristics of ground water.

The capability to predict the movement of various constituents in flowing ground water can be of help in (Konikow, 1970)

(1) Planning and designing projects to minimize ground water contamination.

(2) Estimating spatial and temporal variations of concentrations of inorganic constituents.

(3) Estimating the time of travel between a source of contamination and a discharge point such as a stream, spring or well.

(4) Designing an effective and efficient monitoring system.

(5) Evaluating the physical and economic feasibility of alternative reclamation plans for removing contaminants from an aquifer and/or preventing the contaminants from spreading.

The purpose of a digital computer quality model is to compute the concentration of a dissolved constituent in an aquifer at any specified place and time. Since the movement of contaminants depends to a large degree on the velocity of ground water flow, it is a necessary prerequisite that the flow system be simulated. This, in essence, requires that a two or three-dimensional model of the flow system be calibrated before a reliable quality model can be developed.

A model which includes quality considerations must solve two simultaneous partial differential equations. One is the equation of flow (such as equation 7-1), from which ground water velocities are obtained, and the second is the solute-transport equation, describing the concentration of a dissolved constituent in the ground water (Konikow, 1970). It is important to note that the finite-difference and finite-element approximations of the flow equations do not directly yield ground water velocities. The velocities calculated by these methods are apparent velocities of the flow regime. Consider the discharge, Q_2, through the cross-sectional area, 2, of Figure 7-1. The apparent velocity is the discharge, Q_2, divided by the cross-sectional area, 2. The average seepage velocities (velocities of flow through the pore spaces of the aquifer material) necessary in quality simulations are determined by taking into account the effective porosity (the fraction of the gross cross-sectional area of the saturated earth material representing the portion through which flow occurs) according to

$$V_i = \frac{K_{ij}}{n} \frac{\partial h}{\partial x_j} \qquad i,j = 1,2 \qquad (7\text{-}9)$$

where V_i is the seepage velocity in the i-direction (LT^{-1})
K_{ij} is the hydraulic conductivity tensor (LT^{-1})
n is the effective porosity (dimensionless)

Although it is not necessary to fully understand equation 7-9, what is important is that an additional physical characteristic of the aquifer, effective porosity, must be determined at each node in the system when including quality of ground water in the simulation.

The solute-transport equation, generally used to describe transport and dispersion of a given dissolved chemical constituent in flowing ground water, involves the following considerations:

(1) Dispersion characteristics of the porous medium
(2) Effects of convective transport (function of the seepage velocity)
(3) Concentration of dissolved chemicals at a particular source of recharge or discharge (such as wells, rivers, canals, etc.)
(4) All chemical reactions affecting the chemical constituents of interest

Item 4 above may be eliminated from consideration in the case of a conservative, nonreacting constituent. (Conservative constituents are those considered to have little or no reaction to their present environment. Nonconservative constituents, on the other hand, are those that react to some degree with the chemical composition of the rocks with which they have been in contact, the temperature, the pressure, the duration of contact, the materials already in solution, etc.) From the above discussion, it is apparent that a significant amount of additional data is required when quality considerations are included in the modeling effort.

Coupled computer programs are available to model both the flow system and transport of chemical constituents. They are applicable to unconfined, heterogenous and anistripic aquifers either in two or three space dimensions. Although there have been several successful applications involving quality, at the present they are rather limited in scope and still, in many respects, in a developmental state (Konikow, 1970; Konikow, et al., 1974).

With respect to the AGUA, it would appear that only a few possibilities exist in regard to quality modeling based on the successful applications for somewhat similar basins. (This is not to say that successful simulations of other chemical constituents are not possible at present but that they have not been successfully applied to a degree that would warrant practical consideration). Of those successful applications (mostly two-dimensional systems), the assumption was made that no chemical reactions occurred between the chemical constituent of interest and the aquifer or soil materials that would affect the concentration. The solute-transport equation in this case reduces to a consideration of dispersion, convective transport and the concentration of dissolved chemicals for various sources of recharge or discharge. Although the above assumption limits the quality analysis to relatively conservative (nonreacting) chemical constituents, reasonable simulations have been made for low-level radioactive wastes and dissolved solid concentration variations (Konikow, 1970; Konikow, et al., 1974). Of the latter, an analysis of dissolved solid concentrations or salinity increases of the ground water resource due to irrigation practices could be simulated.

In summary a coupled ground water flow quality model as applicable to AGUA would calculate the head distribution in the aquifer at the end of each computation period (time step). The hydraulic gradients determined from the new water table elevations would then be used to compute seepage velocities through the aquifer. The changes in concentration due to dispersion and convective transport of the chemical constituents during the time step would be computed next based on ground water velocities and the concentration gradients in the aquifer at the beginning of the simulation period.

Since two-dimensional flow and quality models appear reasonable for AGUA, the following remarks are applicable to a coupled two-dimensional flow-quality simulation (assuming conservative chemical constituents). In addition to that discussion made previously for modeling flow systems, and which are applicable now, quality simulation involves consideration of many other conditions. Constant concentration boundaries and the concentration at each node in the model must be specified for those time periods utilized in the calibration process. The finite-grid system (if used) developed must be based on both quantity and quality considerations. Calibration of the model now includes matching concentration changes over time and space; and the data requirements for inclusion of quality are, in general, noted below:

(1) A map of effective porosity values for the area included in the ground water study
(2) A map of the dispersivity characteristics of the porous medium
(3) Concentrations of the chemical constituents of interest in the aquifer for each time period used in the calibration process
(4) Concentrations of the chemical constituents of interest of all applied water (precipitation, irrigation water, surface water, wastewater effluent, etc.)

Several points should be emphasized at this time in regard to the computer programs available for ground water modeling and which might be considered for the AGUA.

The two-dimensional computer programs consider flow in the horizontal plane only. Vertical flow or the vertical component of flow cannot be handled directly. Various modifications have been incorporated in the two-dimensional systems to handle vertical components, but the added complications make it difficult to apply in the real sense. At present it would appear that a two-dimensional model could adequately simulate the ground water flow system of the AGUA. The one problem which might arise and which could introduce significant errors in the calibration process, is the possibility that the major transmissivity tensor (vector) is inclined to the plane containing the grid or element system. This situation could occur if stratified layers of valley-fill material exist and if they slope away from the land surface rather significantly. In this case the value of transmissivity in the two-dimensional system will have to be adjusted to compensate for the vertical component and the adjusted values will no longer reflect the real system. If the adjustment is extreme then calibration of the model may be unattainable.

Although finite-element methods offer distinct advantages over finite-difference methods, they are at present not well documented nor have they been widely applied to ground water systems similar to the AGUA. The U.S. Geological Survey in their ground water modeling efforts for the San Bernardino Valley Municipal Water District, will utilize both methods and compare the results.

In either the two or three dimensional system the drawdown in an individual well is not computed directly. The models compute a hydraulic head that represents the average head over an elemental area. Various analytical techniques can be used to compute the approximate drawdown in a well based on the average hydraulic head (Trescott, et al., 1976).

If the objective of a modeling effort in the AGUA is to simulate the ground water flow system; then at present a finite-difference two-dimensional model would appear to be the simplest model that will yield adequate results. If quality is an objective, then it must be remembered that the flow system be reasonably simulated before a reliable quality model can be developed.

A Digital Computer Model for the AGUA

Discussions in this section support the conclusion that a two or three dimensional digital model of the AGUA ground water flow system could be developed successfully. Although the area of the ground water basin to be simulated would depend upon the specific objectives of a particular study, it appears that adequate data could be assembled (regardless of the size of the area within AGUA) to adequately calibrate a flow model. In the case of a coupled flow-quality model, it's development is less certain because of limited availability of documented computer programs, the inability at present to simulate reactive chemical constituents, and only a small number of practical situations that have been adequately simulated. It should be emphasized that before a reliable solute-transport model could be developed, a model of the flow-system must be calibrated. This latter fact suggests that a flow model could be undertaken before incorporating quality aspects. In the time that it might take to calibrate the flow model, advances in the field of quality simulation may be such as to warrant its consideration at a future date. With this in mind a computer program should be selected that is adaptable to quality as well as flow considerations.

Reasons for Modeling. Several reasons for utilizing a digital computer model in the AGUA are discussed below and provide the basis for judging the utility of undertaking a modeling effort.

(1) Determine quantitatively and spatially recharge due to irrigation canals, wastewater treatment facilities, streams, etc.

(2) Evaluate effectiveness of basin management plans on the water resource both quantitatively and qualitatively

(3) Investigate impacts of wastewater discharges on the system

(4) Study effectiveness of replenishment programs

(5) Evaluate pumping programs
   a. Economic optimums
   b. Hydraulic impacts

(6) Determine sensitivity of assumptions in both modeling techniques and input data

(7) Help design monitoring and surveillance programs

(8) Learn more about the behavior of the ground water basin , and

(9) Encourage a businesslike approach to development and management of water resource data.

In analyzing reasons for considering a digital computer model, it should be noted that the digital model has the capability of describing the total system in quantitative terms; and interrelationships between components of the system and stresses on the system can be considered simultaneously. The real potential of a model of this type arises when a ground water flow system has been reasonably calibrated and verified. At this point in time the model can be utilized for rapid evaluation of multiple alternatives and possibly coupled with quality, economic and rainfall-runoff models.

Costs for Developing a Digital Computer Model. Since the objectives of any particular modeling effort for the AGUA are, in general, not known, definitive cost estimates are not possible. It is possible, though, to relate costs of other ground water modeling efforts in similar basins to those that might be contemplated for the AGUA.

A ground water modeling effort (to predict ground water levels) developed by the Kern County Water Agency in cooperation with the California Department of Water Resources began in April of 1967 (Kern County Water Agency, 1974, 1974 and 1977). The maximum obligation of the water agency under the initial five year agreement was $250,000. Included within the obligation was the stipulation to provide personnel necessary to acquire and tabulate data relative to land and water use during historic times (approximately 115 man-months) and to provide computer services. The model (a modification of a two-dimensional link-node computer program developed by the California Department of Water Resources) simulated a flow system consisting of confined and unconfined aquifers covering approximately 2000 square miles. Each elemental area of the polygonal grid system contained approximately 9 square miles.

The City of Modesto in a 50-50 cost sharing effort with the U.S. Geological Survey contracted to develop a two-dimensional (finite-difference) ground water model of the unconfined aquifer in and near the City of Modesto, California (Page, 1977). The model encompasses about 542 square miles utilizing a variable rectangular grid system. The City's estimated cost to date is approximately $200,000 which includes personnel necessary for the data collection effort. The model is expected to be available as a management tool around 1979-1980 after additional data collection and refinements to the existing model are made. (The effort will take about seven years with a total cost to the city of about $250,000).

The San Francisco District, U.S. Army Corps of Engineers, contracted with the U.S. Geological Survey to develop a ground water model for the Salinas Valley area of California (U.S. Geological Survey, 1978). The area of interest was approximately 600 square miles and consists of confined and unconfined conditions within the aquifer system. Finite-element techniques are used to model the aquifer in both two and three space dimensions. The contract also included the development of a ground water quality model (a coupled flow-quality model) to simulate the transport of conservative chemical constituents and tests of future alternatives involving both flow and quality. The time involved was estimated as three years with a total cost to the San Francisco District of $300,000.

Although the area that a ground water model might encompass in the AGUA is not known it would probably be much less than the study limits. If one extends the idealized boundaries of the aquifer as defined in previous studies (Reeder, 1967) the area would probably be about 1400 square miles. Then depending on the interests of a particular modeling effort (whether to determine the effects of pumping on Rio Grande flows, quality of water in the immediate vicinity of the Rio Grande, etc.), the area covered would still be significantly less than that.

An analysis of the costs of similar studies including those previously cited, indicates that the cost of data collection, analysis and interpretation is about 40 percent of the cost associated with the development of the ground water flow model. (Of course, the data collection effort is dependent on the difficulties involved in calibration and on the following sensitivity analyses). A summary of estimated costs and times (which might be overlapping) associated with a ground water mdoeling effort in the AGUA is given below:

	Time (year)	Cost
(1) Data collection, analysis and interpretation	1-3	$40,000
(2) Development of ground water flow model		
Two-dimensional (Finite-difference or finite-element)	2-4	100,000
		$140,000

The total cost of $140,000 represents the cost of developing a flow model adequate for general planning purposes (assuming a computer program can be acquired from some agency or organization). It is expected that continued data collection and refinement of the model will be necessary as various sensitivity tests are made and new data becomes available.

If water quality is a consideration, then the total cost of a model is expected to increase significantly. A summary of the estimated total cost and time associated with a coupled ground water flow and quality model are indicated below:

	Time (year)	Cost
(1) Data collection, analysis and interpretation	2-4	$75,000
(2) Development of a ground water flow and quality model (conservative chemical constituents)		
Two-dimensional (Finite-difference or finite-element)	3-5	175,000
		$250,000

Although the costs should be viewed as preliminary in nature, there is one consideration that is important to note. The U.S. Geological Survey can enter into cooperative (50-50 cost sharing) agreements with local agencies (such as cities, water districts, etc.) to model the ground water basins of interest. For an agency contemplating modeling of the AGUA aquifer system, the cooperative effort should be considered not only in regard to funding but also in regard to the technical capabilities of the U.S. Geological Survey in the field of ground water modeling.

Guidelines for the Development of a Ground Water Model. The following are important considerations for determining when a digital computer modeling effort should be initiated.

(1) Evidence of the need for effective ground water management. It is advantageous to begin data collection and model development before critical problems develop so that information provided by a model can assist in preventing such problems. A properly calibrated and verified model can be an important tool in effective ground water management. In situations where problems have already developed a model can be effective in analyzing the problems, exploring alternative solutions, and in minimizing the severity of such problems.

(2) An interested, capable, responsible public agency and staff. A good example of this is the San Bernardino Valley Minicipal Water District (San Bernardino, California). Although this agency was one of several agencies operating within the basin and without complete legal jurisdiction over the activities of the other agencies, they felt it was still in their best interests and in the bests interests of all concerned to develop a ground water model and to devise a data collection and management system for the entire basin.

(3) An adequate budget and time schedule.

An investigation of numerous ground water model studies involving unconfined aquifer systems somewhat comparable in size to the AGUA, suggests a range of costs between $150,000 to $400,000 depending on the complexity of the model and the data available. In most of those studies an intensive data collection effort spanned two to four years.

(4) Availability and use of the proper technology
Computer programs are available for modeling ground water systems. For two and three space dimensions ground water flow systems have been modeled with consistently satisfactory results over the last decade (Pinder, et al., 1968; Kern County Water Agency, 1977; Konikow, et al., 1974). The ability to model quality of ground water (the capacity to predict the movement and concentration of dissolved chemicals) is still in a transitional stage. Although there have been numerous studies in which the movement and concentration of conservative chemicals (non-reacting), particularly dissolved solids, have been satisfactorily simulated (Konikow, et al., 1974) the capability to model the movement of organic or nonconservative (reactive) chemicals is still very much in the developmental stage (Konikow, 1970). In the case of combined models, such as coupled ground water/economic systems and coupled ground water/rainfall-runoff models, they are still in the developmental and verification stages.

(5) Sufficient data and information
Ground water modeling efforts to date involve an analysis (collection and interpretation) of existing data, the collection of new data, and data management programs. The same procedure is expected for the AGUA. (It should be noted that one of the objectives of developing a model is to pinpoint areas where additional information is required and based on a sensitivity analysis, to determine which data needs to be determined more accurately).

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