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Publication Date

1977-05-20

*Presented at the IBM Seminar on Regional
Groundwater Hydrology and Modeling,
Venice, Italy, May 25-26, 1976*

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May 20, 1977

Lawrence Berkeley Laboratory University of California/Berkeley
Prepared for the U.S. Energy Research and Development Administration under Contract No. W-7405-ENG-48

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RECENT DEVELOPMENTS IN MODELING GROUNDWATER SYSTEMS

By

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ABSTRACT

This paper reviews the developments in the mathematical modeling of groundwater systems over the past decade. The first part of the paper is devoted to a description of the physics of the different types of problems that are of interest in hydrogeology and a statement of the related initial-boundary-value problems. The various numerical techniques that have been employed to solve the governing equations are discussed in the second part. In the third section a few typical case histories are presented to illustrate the trend of progress that has occurred in the application of mathematical modeling to actual field problems.

INTRODUCTION

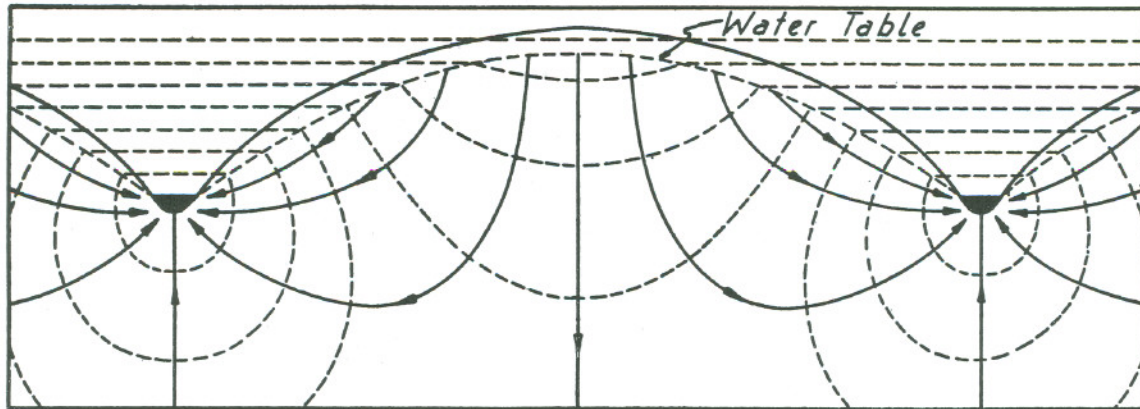
This seminar on Regional Groundwater Hydrology and Modeling is timely, as it provides us a motivation to pause and take stock of our repertoire concerning a very rapidly growing branch of hydrogeology, namely, mathematical modeling. The aim of regional groundwater modeling is to represent the natural groundwater system by an equivalent abstract model in order to explain or understand the behavior of the system. The conceptual basis for the abstract model is the law of mass conservation. The very nature of the model is that it is always less complete than the real system (Domenico, 1972). Models, therefore, vary widely in the degree to which they approximate the real system. A major constraint governing the gap between the real system and the mathematical model is the availability of appropriate tools to obtain tractable results or solutions from the latter.

Until about a decade ago, the mathematical tools available for modeling groundwater systems were restricted to either analytical methods, capable of yielding practical solutions for simple systems, or to numerical methods, severely restricted in power for want of fast computing ability. For a long time, therefore, the major effort in mathematical modeling was directed towards the solution of initial-boundary-value problems expressed as partial differential equations. To obtain these solutions a variety of classical mathematical tools such as separation of variables, integral transforms, Green's functions, conformal mapping, and velocity hodographs were used. From the simple model for steady flow in a radial sys-

tem (Thiem, 1906), to the currently available models of complex systems such as multilayered leaky aquifer systems or unconfined systems characterized by delayed drainage or flow systems with simple fractures, these models lead to solutions of increasing complexity (e.g. Aravin and Numerov, 1965; Bear et al., 1968; Carslaw and Jaeger, 1973; Hantush, 1964; Polubarinova-Kochina, 1962). It seems reasonable to assume that we are very close to the limits of these models in being able to represent real systems.

In the recent past, many workers in the field of hydrogeology have directed their attention to the use of numerical methods, which enable one to handle the complexities of real systems that cannot easily be handled by the classical analytical methods. The practical use of numerical methods has been mainly possible due to the increased availability of fast computing machines. It is with these numerical approaches that this paper is mainly concerned.

Although Meinzer (1923) used the classical geological approach to observe and define the principles of regional groundwater flow over 50 years ago, it was Hubbert (1940) who employed potential theory to define the mathematical foundations of groundwater motion. Hubbert demonstrated its applicability with some simple examples such as the one reproduced in Fig. 1, where the flow of water in a steady unconfined system is represented. In the field of soil physics, which is closely allied to hydrogeology, the potential-theory ap-



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Fig. 1. Pattern of groundwater flow in a simple, steady, unconfined system (Hubbert, 1940).

proach even predates Hubbert's work as evidenced by the classical investigations of Buckingham (1907) and Richards (1931). Surprisingly, Hubbert's powerful ideas lay dormant for a considerable period, and it was not until the early 1960s that his ideas were put to practical use by Canadian hydrogeologists, notably Toth (1962), Meyboom (1962), and others. These studies, in addition to opening up a new perspective in studying regional groundwater systems, also led to the practice of using nested piezometers for observing vertical movement of groundwater within a groundwater basin. These studies also led to the identification of different components of the hydrogeologic system (recharge and discharge areas, base flow) and provided a framework for studying the evolution of water chemistry within the basin.

Toth (1962), who set out to study models of small groundwater basins, used the analytical approach of separation of variables and hence was severely limited in extending his results to more general cases. About the same time, Fayers and Sheldon (1962) employed the finite-difference approach to the study of steady-state movement of fluids in geologic basins. Since the contributions of these early workers, numerical modeling of regional groundwater systems has become a standard tool in the hands of hydrogeologists.

In this paper, we will summarize the highlights of activities within the last 10 years relating to regional groundwater modeling. We will begin with a general statement of the problem of regional groundwater modeling and then examine how the problem is to be solved by different techniques. In this way, we will bring together the various powerful techniques of simulation that have evolved through the investigations of many workers. We will then consider the similarities, dissimilarities, advantages and disadvantages of these simulations. This paper is thus divided into three sections:

- Discussion of the physics of regional groundwater models
- Examination of the methods employed in obtaining numerical solutions
- Review of a few typical case studies

In the broadest sense, regional groundwater modeling should consider the transport of solutes. Further, it should also be extended to include the nonisothermal phenomena occurring in geothermal systems. However, we will restrict the scope of this work only to the hydrodynamics of isothermal groundwater systems.

In a rapidly developing subject such as regional groundwater modeling, it is difficult to include an exhaustive literature search. The references cited here are by no means comprehensive. In a recent work Prickett (1976) presents an excellent review of the available literature on groundwater modeling.

PHYSICS OF REGIONAL GROUNDWATER MODELS

Conceptual Foundation

Most groundwater systems exist under dynamic conditions. It is therefore advantageous to direct our attention to the general problem of non-steady flow and consider the steady-state system as a limiting case of the nonsteady system. The conceptual foundation of regional groundwater movement lies in the law of mass conservation. For any finite subregion of the flow region, the equation of mass conservation can be expressed by*

$$\rho_w \nabla \cdot \mathbf{q} - \int_{\Gamma} \rho_w \mathbf{q} \cdot \mathbf{n} d\Gamma = \frac{\partial M_w}{\partial t} \quad (1)$$

Equation 1 is subject to the nature of the initial state of the system as well as the conditions on the boundaries separating the system from its ambient surroundings. For practical applications it is necessary to rewrite (1) in terms of a convenient dependent variable which in groundwater hydrology is the easily measured quantity, hydraulic head,

$$h = z + \psi \quad (2)$$

where

$$\psi = p / \rho_w g \quad (3)$$

* See Nomenclature for definition of terms.

For saturated flow problems it is convenient to use h as the dependent variable, whereas for problems including unsaturated flow or problems including system deformation, it is necessary to decouple the gravitational and pressure components of h and use ψ as the dependent variable. Before introducing the dependent variable, we shall adopt Darcy's law in the form (Philip, 1969)

$$\vec{q}_r = -K \nabla h \quad (4)$$

Inserting (4) into (1) and assuming, on empirical grounds, that M_w is a function only of h , we obtain

$$\rho_w G V + \int_{\Gamma} \rho_w K \nabla h \cdot \vec{n} d\Gamma = \frac{dM_w}{dh} \frac{\partial h}{\partial t} \quad (5)$$

The amount of water contained in a finite subregion of volume V is given by

$$M_w = \rho_w V S \quad (6)$$

We therefore define a term called the "fluid mass capacity" of the subregion [Narasimhan and Witherspoon, 1976b]

$$M_c = \frac{d}{dh} [\rho_w V S] = V S \frac{d\rho_w}{dh} + \rho_w S \frac{dV}{dh} + \rho_w V \frac{dS}{dh} \quad (7)$$

Physically, M_c represents the amount of fluid mass that the finite subregion can absorb when the average head within the system changes by unity. The general equation of transient groundwater motion therefore takes the form

$$\rho_w G V + \int_{\Gamma} \rho_w K \nabla h \cdot \vec{n} d\Gamma = M_c \frac{\partial h}{\partial t} \quad (8)$$

Equation 8 is in an integral form. It is more customary in the literature to express (8) in a volume-normalized differential form. Thus, we shall first define a quantity "specific fluid mass capacity" as $m_c = M_c / V$, and then divide (8) by V and let the finite subregion become arbitrarily small to obtain

$$\rho_w G + \text{div} (\rho_w K \nabla h) = m_c \frac{\partial h}{\partial t} \quad (9)$$

where divergence is defined by (Sokolnikoff and Redheffer, 1966)

$$\text{div} \vec{q}_r = \lim_{V \rightarrow 0} \frac{1}{V} \int_{\Gamma} \vec{q}_r \cdot \vec{n} d\Gamma \quad (9a)$$

Under conditions when K and m_c are strongly dependent on h , as in the case of unsaturated flow, it is mathematically more convenient to use moisture content θ as the dependent variable instead of h . Thus, soil physicists often use the governing differential equation

$$\rho_w G + \text{div} (\rho_w D \nabla \theta) = \frac{\partial \theta}{\partial t} \quad (10)$$

where

$$D = \frac{K}{\theta} \frac{dh}{d\theta} \quad \text{and} \quad \theta = nS$$

Equation 13 is generally of limited use since it is applicable only to systems composed of a single material (Klute, 1972).

For steady-state flow we let $\partial h / \partial t = 0$ and (9) reduces to Poisson's equation

$$\text{div} (\rho_w K \nabla h) = -\rho_w G \quad (11)$$

and in the absence of sources or sinks (11) further reduces to the Laplace equation

$$\text{div} (\rho_w K \nabla h) = 0 \quad (12)$$

In applying (8) to actual systems, the equation is appropriately modified to accommodate the special dependences of K and M_c on h or to handle special conditions on the boundary. We will now proceed to examine the application of (8) to realistic systems, starting with the simplest case.

Confined Systems

The simplest system to consider is one in which the flow region is fully saturated and the material coefficients K and M_c are independent of time. In such a system, M_c is governed only by the compressibility of water and that of the porous medium. As shown by Domenico (1972, p. 220), for fully saturated confined systems,

$$\rho_w G V + \int_{\Gamma} \rho_w K \nabla h \cdot \vec{n} d\Gamma = V \gamma_w (\alpha + n\beta) \frac{\partial h}{\partial t} \quad (13)$$

The quantity $S_s = \gamma_w (\alpha + n\beta)$ is often referred to as specific storage in groundwater hydrology. Many workers have used (13) for modeling confined groundwater systems with fixed geometry (e.g. Fayers and Sheldon, 1962; Pinder and Bredehoeft, 1966; Javandel and Witherspoon, 1968; and Prickett and Lonnquist, 1971). Equation 13 has also been extended by some to include unconfined systems with the assumption that the position of the water table is known and fixed (e.g., Tysen and Weber, 1964; Freeze and Witherspoon, 1966). The source term in (13) has been used by different workers to simulate the effects of production wells, leakage from aquitards and streams, transfer of water to the atmosphere through evaporation, and infiltration due to rainfall (e.g., Prickett and Lonnquist, 1971).

The chief limitations of (13) are twofold. The first is that it ignores flow in the unsaturated zone. Secondly, it assumes a constant value of S_s , an assumption which may not be appropriate for systems experiencing large head changes over prolonged periods of time or for systems undergoing land subsidence. Since soil deformation is related to stress changes induced by variations in pore fluid pressure, Equation 13 cannot effectively handle time-dependent changes in S_s unless gravity is decoupled from fluid pressure and due consideration is given to the skeletal stress field.

The Free-Surface Approximation

Hydrogeologists and civil engineers often choose to neglect modeling the unsaturated zone so as to avoid the computational difficulties inherent in taking into account the complex dependence of K and M_c on the pressure head ψ . Instead, using suitable approximating assumptions, the effect of the unsaturated zone is replaced by an equivalent boundary condition.

In the case of steady seepage in an unconfined system, it is often convenient to assume that the flow region is saturated, but that the exact location of the free surface is unknown. The mathematical problem then reduces to one of determining the position of a part of the boundary of the flow region (free surface) by trial and error, using the following boundary constraints

$$\begin{aligned} h &= \xi \\ \text{and} \quad \underline{K} \nabla h \cdot \vec{n} &= In_3 \end{aligned} \quad \text{on the free surface.} \quad (14)$$

This approach has been employed by Taylor and Brown (1967), Jeppson (1968), Neuman and Witherspoon (1970), Remson et al. (1971), Cheng and Li (1973), France (1974) and others.

In the case of nonsteady flow with a free surface, the free surface continuously changes position. To handle this feature, the simplifying assumption is made that the water is instantaneously released from the region through which the free surface is given by (Bear et al. 1968; Neuman and Witherspoon, 1971)

$$\begin{aligned} h &= \xi \\ \text{and} \quad \underline{K} \nabla h \cdot \vec{n} &= (I - S_y \frac{\partial \xi}{\partial t}) n_3 \end{aligned} \quad \text{on the free surface.} \quad (15)$$

In most free-surface problems it is customary to assume that the saturated porous medium is rigid, that water is incompressible, and that the saturated flow region obeys the Laplace equation.

An added simplification used by civil engineers is the Dupuit (1863) assumption. That is, the hydraulic head is constant along any vertical line in the aquifer, and water moves only horizontally within the saturated zone.

For steady-state flow, the Dupuit assumption leads to the well-known Forchheimer equation (Prickett, 1975)

$$\frac{\partial^2 (h^2)}{\partial x^2} + \frac{\partial^2 (h^2)}{\partial y^2} = 0 \quad (16)$$

For nonsteady flow in a nonhomogeneous-isotropic aquifer, the Dupuit assumptions lead to (Prickett, 1975)

$$\frac{\partial}{\partial x} (Kh \frac{\partial h}{\partial x}) + \frac{\partial}{\partial y} (Kh \frac{\partial h}{\partial y}) = S_y \frac{\partial h}{\partial t} \quad (17)$$

Equation 17 is also known as the Boussinesq equation and has been used by Pikul et al. (1974).

In writing (15) it was assumed that water is instantaneously released from storage in the region through which the water table is falling. To be more realistic, Boulton (1954) introduced the concept of delayed yield from storage to take into account the slow drainage of water from the unsaturated zone. The delayed-drainage concept has since been examined in detail by Neuman (1972), Streltsova (1972) and others.

Saturated-Unsaturated Flow

More realistic than the free-surface approximation is a groundwater flow model, which simul-

taneously considers flow in the saturated as well as the unsaturated zones. In general, saturated-unsaturated flow involves the consideration of two phases: water and air. A rigorous modeling of saturated-unsaturated flow should therefore involve setting up two mass conservation equations, one for water and one for air (Morel Seytoux, 1973). However, the model is usually simplified with the assumption that the air phase is continuous in the porous medium, and is at atmospheric pressure, thereby neglecting the mass-conservation equation for air.

The saturated-unsaturated flow equation differs from (13) in two respects. First, $\underline{K}$ is a strong function of ψ in the unsaturated zone, and second, it includes a desaturation coefficient, $dS/d\psi$ in the fluid mass capacity term. Thus the saturated-unsaturated flow equation becomes (Freeze, 1971)

$$\begin{aligned} \rho_w \underline{GV} + \int_{\Gamma} \rho_w \underline{K} \nabla h \cdot \vec{n} d\Gamma \\ = V[\rho_w S(\alpha + n\beta) + \rho_w n \frac{\partial S}{\partial \psi}] \frac{\partial \psi}{\partial t} \end{aligned} \quad (18)$$

in which $\underline{K}$ as well as $\partial S/\partial \psi$ are strong functions of ψ , characterized by hysteresis. Equation 18 is inherently nonlinear due to the variability of the material coefficients with ψ . It is often customary to assume that n is constant in the unsaturated zone and that $S_s = (\alpha + n\beta)$ is constant in the saturated zone. Then, neglecting small changes in ρ_w , we obtain the simple relation (Neuman, 1973b)

$$\underline{GV} + \int_{\Gamma} \underline{K} (z + \psi) \cdot \vec{n} d\Gamma = V[S_s + C] \frac{\partial \psi}{\partial t} \quad (19)$$

where $C = \frac{\partial \theta}{\partial \psi}$.

Equation 18 is sometimes further simplified (Vauclin et al., 1975) by assuming that the saturated zone is incompressible. Thus

$$\underline{GV} + \int_{\Gamma} \underline{K} \nabla (z + \psi) \cdot \vec{n} d\Gamma = VC \frac{\partial \psi}{\partial t} \quad (20)$$

Consideration of unsaturated flow leads to some special boundary conditions involving the seepage face and the atmospheric boundaries. The seepage face is a boundary on which (Cooley, 1971; Neuman, 1973b; Narasimhan, 1975; Vauclin et al., 1975) $\psi = 0$ and further, the flux along the outer normal to the seepage face, $\underline{K} \nabla (z + \psi) \cdot \vec{n} > 0$, meaning that flux can only leave the system across a seepage face.

Water can be lost from an unsaturated soil to the atmosphere either by evaporation or by evapotranspiration (Neuman, et al., 1975). The maximum amount of water that the atmosphere can remove from the soil is equal to the sum of potential evaporation and potential evapotranspiration, which must be determined from micrometeorological data. In addition, there also exist lower limits for the pressure heads that can develop either at the dry soil surface or at plant roots. The soil atmosphere boundary is therefore neither a prescribed potential boundary nor a prescribed flux boundary, but is one on which an upper bound for flux and a lower bound for potential are prescribed.

An infiltration boundary is another boundary of interest. If the rate of infiltration at the surface exceeds the ability of the soil to transmit water, as determined by its saturated permeability, then part of the surface addition must be lost as runoff. Thus, an infiltration boundary has an upper limit for boundary flux.

The saturated-unsaturated models described above are of considerable practical use in representing materials of moderate to high saturation. However, the deficiency of these models (Equations 18-20) lies in the fact that they do not give due consideration to the mechanics of soil deformation.

Deforming Porous Media

Accurate modeling of soil deformation is important from the viewpoint of land subsidence due to groundwater withdrawal, as well as for considerations of long-range groundwater management. Experience with the behavior of unconsolidated soils suggests that soil properties such as compressibility and permeability may undergo nonreversible changes with time due to the nonelastic response of the soil to changes in loading (Gambolati and Freeze, 1973; Helm, 1974). As a result, both K and α in (13) become nonlinear coefficients. These nonlinearities are governed by the distribution of skeletal stresses in the soil and hence, in order to duly account for these nonlinearities, one must incorporate the stress field into the governing equation. In considering soil deformation in regional groundwater systems, the changes in regional tectonic stresses are generally ignored and the total stress on the system is assumed invariant in time. However, due to changes in pore fluid pressure caused by water movement, the skeletal stresses change with time causing soil deformation. The primary conceptual necessity in modeling deformation is therefore a relation between pore fluid pressure and skeletal stress.

Soil deformation is generally a three-dimensional phenomenon and a rigorous solution of the problem should consider solution of two independent governing equations -- one for fluid flow and another for stress-strain behavior, which are coupled through a criterion that assures compatibility of volume change (see for example, Sandhu and Wilson, 1969). However, in regional groundwater modeling, the consideration of the general stress-strain equation is usually avoided on grounds of effort and economy. Instead, making use of the basic concept of one-dimensional consolidation theory of Terzaghi, soil deformation is handled in an approximate fashion with the help of a single fluid-flow equation. The one-dimensional consolidation theory has been used for modeling groundwater systems by Gambolati and Freeze (1973), Helm (1975) and Narasimhan (1975).

The one-dimensional theory of deformation is ideally suited for systems in which lateral strains are negligible and all the deformation occurs in the vertical direction. Fundamental to this theory are the concepts of effective stress, σ' and its relation to pore water pressure given by

$$\sigma' = \sigma - \gamma_w \psi \quad (21)$$

However, some petroleum engineers (Robinson and Holland, 1970) believe that only part of the pore water pressure (the concept of boundary porosity) may influence σ' . Similar ideas have also been expressed by Bishop (1959) and McMurdie and Day (1960) in attempting to relate negative pore pressure and effective stress in the unsaturated zone. Thus,

$$\sigma' = \sigma - \chi \gamma_w \psi, \quad 0 \leq \chi \leq 1 \quad (22)$$

The parameter χ can especially be a function of ψ in the unsaturated zone. Assuming $\sigma = \text{constant}$ and $\chi = \chi(\psi)$, we obtain

$$\frac{d\sigma'}{d\psi} = -\gamma_w \chi' \quad (23)$$

where

$$\chi' = \left[\chi + \psi \frac{d\chi}{d\psi} \right] \quad (24)$$

The principal task in applying (8) to a deformable porous medium is to evaluate the quantity dV_v/dh occurring in the fluid mass capacity term on the right hand side of (7). Since $h = z + \psi$ and since both z and ψ may vary with time in a deformable porous medium, it is advantageous to make the reasonable assumption that z does not vary appreciably in any given interval of time and hence can be handled as a temporal step function. Then, in the light of (24) we can write

$$\frac{d(V_v)}{dh} = \frac{d(V_v)}{d\psi} = \frac{d(V_v)}{d\sigma'} \frac{d\sigma'}{d\psi} = -\chi' \gamma_w \frac{d(V_v)}{d\sigma'} \quad (25)$$

Another point to remember here is that Darcy's law describes the velocity of water relative to the velocity of grains (e.g. Philip, 1969). The dependence of Darcy's law on grain velocity as well as the fact that the elemental volume itself varies with time, requires a precise definition of the nature of the volume element for which the conservation equation is written and the reference coordinate system. These questions have been examined by Cooper (1966), Smiles and Rosenthal (1968), Philip (1969), Verruijt (1969), Gambolati (1973a,b), Cooley (1975) and others. Essentially, the problem can be approached in two different ways: (a) the Eulerian approach using a fixed coordinate system, in which the bulk volume of the elemental volume is constant in time; or (b) the Lagrangian approach using a material coordinate system, in which the elemental volume has constant volume of soil particles, and in which the soil particles remain at rest. Jacob's (1950) classical development of the equation of groundwater flow, as pointed out by De Wiest (1969), related to a hybrid elemental volume, which was treated in a Eulerian fashion in the space domain and in a Lagrangian fashion in the time domain.

According to Gambolati (1973b), the one-dimensional flow equation for a fixed element in fixed coordinates should read

$$\begin{aligned} \frac{k}{\gamma_w} \frac{\partial^2 p}{\partial z^2} = \{ [(P \frac{d\alpha}{dp} + \alpha) / (1 + \alpha p)] + n\beta \} \cdot \\ \left[\frac{\partial p}{\partial t} + v_g \frac{\partial p}{\partial z} \right] - \frac{k\beta}{\gamma_w} \left(\frac{\partial p}{\partial z} \right)^2 - 2KS \frac{\partial p}{\partial z} \quad (26) \end{aligned}$$

However, the standard groundwater equation (analogous to Equation 13) neglects several terms in (26) and reduces to

$$\frac{k}{\gamma_w} \frac{\partial^2 p}{\partial z^2} = (\alpha + n\beta) \frac{\partial p}{\partial t} \quad (27)$$

Gambolati (1973b) examined the range of validity of (27) and concluded that the standard groundwater flow equation gives satisfactory results in the vast majority of cases and is unreliable only in extremely deformable soils.

In recent works, Narasimhan (1975) and Narasimhan and Witherspoon (1976b) have used a material element volume with constant volume of solids and have combined the one-dimensional deformation approach with a general three-dimensional field of fluid flow. In this model of saturated-unsaturated flow in deformable porous media, the governing equation can be expressed in an integral form as

$$\rho_w \nabla V + \int_{\Gamma} \rho_w \nabla V(z + \psi) \cdot \vec{n} d\Gamma = V_s \rho_w [\text{Sep}_{so} \beta g + S_{\gamma_w} \chi' a_v + e \frac{dS}{d\psi}] \frac{D\psi}{Dt}, \quad (28)$$

where $a_v = -de/d\sigma'$ is the coefficient of compressibility used in soil mechanics literature and D/Dt is a material derivative. In this model irreversible or nonelastic soil deformation is handled by using the equivalences

$$a_v = 2.303 \sigma' C_c \quad \text{or} \quad a_v = 2.303 \sigma' C_s,$$

where C_c and C_s are, respectively, Compression Index and Swelling Index of soil mechanics literature (Lambe and Whitman, 1969).

A small but significant point to be considered in uniting the saturated and the unsaturated zones is the release of stored water from the capillary fringe (Narasimhan, 1975; Narasimhan and Witherspoon, 1976b). By definition, the capillary fringe is the region where $\psi_A \leq \psi < 0$, where ψ_A is the so-called air entry value. Physically the soil cannot desaturate unless $\psi < \psi_A$. If, as is customary in the soil physics literature, water is assumed incompressible and porosity is assumed constant, then within the capillary fringe, M_c becomes zero, implying that there is no physical process by which water could be released from storage. As a result, the soil moisture diffusivity K/m_c becomes infinite. One way to reconcile the situation is to assume that flow obeys the Laplace equation in the capillary fringe. However, under certain boundary conditions (as for example, an isolated saturated system beginning to drain), one may not be able to use the Laplace equation in the capillary zone.

A more general way of handling the problem is to consider the material in the capillary fringe to be deformable. In this case, as shown by Narasimhan and Witherspoon (1976b), the soil-moisture diffusivity of soil physics becomes synonymous with the coefficient of consolidation in soil mechanics.

Flow in Fractured Rocks

It is now well established from detailed geological investigations that many groundwater reservoirs are characterized by the presence of one or more systems of fractures. When the rock matrix is poorly permeable or impermeable, these fractures may act as the sole space for storage and water movement. On the other hand, when the rock matrix is permeable, the result is a fractured porous medium. Since fractures are essentially abrupt discontinuities in the reservoir, flow in fractured systems is in certain respects considerably different from that in porous media. For instance, permeability of a fracture is known to be directly related to the aperture size (Snow, 1965; Romm, 1966).

The detail with which flow in fractured rocks is to be modeled is primarily a question of scale. For regional groundwater modeling, it is therefore convenient to replace the fractured system with an equivalent anisotropic medium (Snow, 1969), the anisotropy being caused by preferred fracture orientation. While this approximation may be practically sufficient for the class of problems of interest to the hydrogeologist, there may be situations related to stability of dams or rock slopes and tectonic behavior of faults that warrant a more detailed consideration of fractures. To handle such problems, the fracture must be allowed to open or close in response to stress changes. Flow in fractured systems can therefore be handled only when two equations are solved: one for fluid flow and one for stress-strain. The most general fracture flow model is one in which the fracture is deformable and in which the rock matrix also has some permeability. Currently, these models are used primarily for modeling systems subjected to seismic stresses or groundwater systems controlling civil engineering structures. Mathematical models for simulating flow in fractured rocks have been employed by Louis (1969); Noorishad (1971); Sharp (1970); Gale (1975); and others.

Wellbore Storage and Related Phenomena

Hydrogeologists and petroleum engineers are often interested in modeling phenomena that occur very close to the wellbore. The more important among these phenomena are: wellbore storage, partial penetration, multiplicity of aquifers, fractures, and skin effects.

The investigations of van Everdingen and Hurst (1949) and Papadopoulos and Cooper (1967) have established that the early drawdown and build-up pressure performance of wells may be considerably perturbed by the effects of wellbore storage, if the transmissivity of the aquifer is relatively small in relation to the radius of the wellbore. This perturbation may also extend to some distance away from the wellbore (Jargon, 1976). The effects of partial penetration in wells have been discussed in detail by many workers, e.g. Muskat (1949), Hantush (1964) and others. These investigations show that in the vicinity of a partially penetrating well, pronounced vertical components of flow develop and that the flux rate across the

well varies along the vertical direction. Yet another feature that introduces variation of fluxes along the wellbore is the presence of more than one producing layer, each with differing flow properties.

Perhaps the simplest way to handle the simulation of wellbore storage and to avoid estimating the variation of fluxes along the wellbore is to treat the well as an integral part of the flow region and to set up a mass balance equation for it. The well discharge then becomes a known source term and the fluid mass capacity of the well (M_c) is either equal to its volume per unit length of well casing (if the well has a free water surface) or equal to the product of the total volume of the well and the compressibility of water (if the well is shut in and filled with water). Huang (1973) points out that this simple scheme destroys the symmetry of the matrix of numerical equations and hence is unsuited to direct matrix solution schemes. Alternatively, it is customary to treat the surface of the well as an external boundary of the flow region, to make an initial guess about the drawdown in the well or about the variation of fluxes along the wellbore, and to use an iterative scheme to obtain the correct solution (e.g. Cooley (1971); Huang (1973)).

Closely allied to the problem of simulating the wellbore is that of handling large fractures located close to the wellbore. These fractures may be horizontal or vertical and may or may not intersect the well. Since fractures usually have much higher conductivities than the matrix, the early-time potential field close to the wellbore is dominated by the flow field associated with the fractures. In modeling such fractures, one could treat them either as having zero volume or as having finite volume and deformability. In the former case, the fracture is treated as an external boundary of the flow region over which the well discharge is distributed in a prescribed way. In the latter case, when the fracture has finite volume and deformability, it can often be treated as infinitely conducting, in which case the method of simulating the fracture is very similar to that of simulating wellbore storage, except that the fluid mass capacity M_c of the fracture is equal to the product of its volume and its deformability. For practical purposes, a vertical fracture can be treated as infinitely conductive when the coefficient $a = 2\pi K L_f / 4\pi K_f w_f < 0.1$ (Prats, 1961). When $a > 0.1$, significant potential gradients develop along the fracture length and the fracture would have to be treated as a finite conductivity material.

The hydraulic efficiency of a well (e.g. wellbore damage, choked gravel pack) can often be simulated as a "skin" effect, a concept that is extensively used in the petroleum engineering literature (Matthews and Russell, 1967). The basic idea here is that the excess drawdowns that may occur close to the wellbore due to well losses can be considered equivalent to the effect of a low-permeability skin around the well. The skin factor s is thus a function of the skin permeability and thickness and is given by $s = (K/K_s - 1) \cdot \log_e r_s / r_w$ (Jargon, 1976). Methods of analyzing the effect of fractures and skin effect on flow to

wellbores have recently been reviewed by Ramey (1976).

Statistical Models

Our discussions so far have been based on a deterministic approach in which the properties of the porous medium, such as permeability and fluid mass capacity as well as the other data such as initial distribution of hydraulic heads and boundary conditions, are precisely known. However, natural groundwater systems that result from complex geological processes, are seldom uniform and hence are characterized by a marked variability in spatial properties. Therefore, when a natural groundwater body or some portion of it is characterized as homogeneous or heterogeneous, there is an element of uncertainty associated with such characterizations. In order to properly understand the significance of these uncertainties in relation to their effect on the mathematical model, some workers have recently been turning their attention to the use of statistical techniques.

The statistical approach has been used in groundwater modeling along three broad lines: (a) to correlate and synthesize limited field data prior to setting up a deterministic simulation model; (b) to quantify the uncertainties inherent in the definitions of the homogeneity of soil parameters and to take into account the effect of these uncertainties on the system response; and (c) to examine the foundations of the equation of motion (Darcy's law), which governs the movement of water in soils.

Lippman (1974) applied the short-memory Markov chain process to synthesize the sand-clay sequences encountered in boreholes in an alluvial basin. He then used a Poisson process to generate a two-dimensional fluid-flow model which would be statistically equivalent, insofar as overall fluid flow is concerned, to the real groundwater system. Wu et al. (1973) used a stochastic model to simulate the distribution of permeable materials in various construction sites.

Freeze (1975) points out that it is more realistic to represent the hydrogeologic parameters as frequency distributions over stochastic macroscopic elements than to represent the parameters as simple values. Such frequency distributions, when used in groundwater models, help estimate the confidence limits of the computed system behavior. This investigation, in short, focuses attention on the stochastic nature of the differential equation governing groundwater movement.

A very special feature of modeling porous media flow is that of the scale transformations involved. Whereas the actual flow takes place in the microscopic pores, where the Navier-Stokes equation is valid, the concepts of Darcy's law and permeability used in hydrogeology are macroscopic, average concepts. There is thus a scale transformation of several orders of magnitude between the microscopic and the macroscopic elements. In a recent paper, Bhattacharya et al. (1976) have used the nonhomogeneous Markov process to conclude that the diffusion equation describing groundwater flow is a mathematically rigorous result of a fundamental stochastic hypothesis. Gray and O'Neill (1976)

and Witherspoon et al. (1975) have shown how the macroscopic flow equations can be developed from microscopic considerations using appropriate techniques of averaging.

Inverse Models

The various approaches discussed so far have involved synthetic models in the sense that one must synthesize known data on geometry, material properties, boundary conditions, and initial conditions, and predict the time variations in hydraulic head. From the viewpoint of the hydrogeologist, the chief drawback of the synthetic model is that the material coefficients (permeability and fluid mass capacity) so essential to field applications are usually not accurately known.

In addition to the synthetic models, an analytic approach has also been developed for the inverse purpose of estimating material coefficients based on the known time behavior of a groundwater system. To determine the material properties of the groundwater system, hydrogeologists have traditionally relied almost exclusively on well-test techniques. A major deficiency in such techniques is that they are based on a gross simplification of material properties and flow region geometry. Moreover, well tests are usually of short duration (tests exceeding a few weeks of production are rare), and hence, they do not yield reliable information on the long-range behavior of the system.

Since the late 1960s, interest has steadily grown in using computers to apply inverse models to groundwater systems that are much more general than those considered in any well-test technique. In general, three basic steps can be recognized in setting up these models. These are model selection, parameter estimation and acceptance (Matalas and Maddock, III, 1976). The model that is most widely used in regional groundwater models is the classical parabolic, partial differential equation (9). The inverse problem related to (9) is one of identifying the spatially distributed parameters, principally, the coefficients of transmissivity and storage.

In general, two approaches exist to estimate the distributed parameters: the indirect and the direct approach (Neuman, 1975a). The indirect approach is basically a trial and error method in which an initial guess of the parameters is made, the problem simulated with the model, and the results compared with the known behavior of the real system. If the deviations from reality are unacceptable, the parameters are appropriately adjusted and the simulation repeated. The iterative process is continued until the model deviations are within acceptable limits. The corrections applied to the parameters with each successive iteration can be made either on the basis of empirical criteria or on the basis of formal mathematical procedures, using digital or hybrid computers.

The direct approach to the inverse problem consists in treating the model parameters as dependent variables in a formal inverse initial-boundary-value problem (Neuman, 1973a). Mathematically speaking, the governing equation (9), expressed

in this fashion, is not well posed (Emsellem and deMarsily, 1971). It is also accompanied by the problem of instability (Distefano and Rath, 1975). In the direct procedure the solution is sought by minimizing a linear functional of residual errors with respect to material balance of hydraulic heads, with the aid of linear or quadratic programming.

Although the inverse problem is not well posed mathematically, it can be sufficiently regularized with the use of appropriate physical criteria. Emsellem and deMarsily (1971) thus use a flatness criteria for the solution in addition to the minimization of residuals. In a similar fashion, Neuman (1973a) uses a plausibility criterion to keep the transmissibility values within specified limits, in addition to minimizing the error functional for material balance. In this approach, alternative solutions may be necessary from which the decision maker selects an appropriate choice. Distefano and Rath (1975) formulate the parameter-identification problem as an optimization problem in which the objective to be minimized is a suitable norm of the difference between observed and estimated hydraulic heads at specified observation wells with known time histories.

General Governing Equation

Before passing on to a discussion of the methods of solving the groundwater flow equation, it is desirable to summarize the physics of mathematical models in the form of a single governing equation. Thus, the equation governing saturated-unsaturated flow of groundwater in a medium undergoing one-dimensional deformation may be written as (Narasimhan, 1975; Narasimhan and Witherspoon, 1976b).

$$\rho_w \nabla \cdot \mathbf{v} + \int_{\Gamma} \rho_w \mathbf{k} \nabla (z + \psi) \cdot \mathbf{n} = M_c \frac{D\psi}{Dt} \quad (29)$$

where

$$M_c = V_s \rho_w [\text{Se} \rho_{wo} \beta g + S \gamma_w \chi' a_v + e \frac{dS}{d\psi}] \quad (30)$$

Equation 29 pertains to a material volume element fixed in the solids (deforms the volume element in fixed coordinates) and hence the geometrical parameters V and e as well as the spatial terms occurring in the surface integral are functions of the dependent variable. The governing equation is in general nonlinear with the following functional dependences: $\rho_w = \rho_w(\psi)$, $G = G(\psi, t)$, $\mathbf{k} = \mathbf{k}(\psi)$ and $M_c = M_c(\psi)$. Equation 29 could be expressed as an equivalent partial differential equation by

$$\rho_w G + \text{div } \mathbf{k} \nabla (z + \psi) = m_c \frac{\partial \psi}{\partial t} \quad (31)$$

The initial and boundary conditions to which (29) and (31) are subject are as follows:

Initial Conditions

$$h(x_i, 0) = (z + \psi)(x_i, 0) = H_0(x_i) \quad (32)$$

Boundary Conditions

$$h(x_i, t) = H(x_i, t) \quad \text{on } \Gamma_1 \text{ (Dirichlet)} \quad (33)$$

$$\underline{K} \nabla h \cdot \vec{n} = -v(x_1, t) \quad \text{on } \Gamma_2 \text{ (Neumann)} \quad (34)$$

$$\left. \begin{aligned} h(x_1, t) &= x_3 \\ \underline{K} \nabla h \cdot \vec{n} &> 0 \end{aligned} \right\} \quad \text{on } \Gamma_3 \text{ (seepage face)} \quad (35)$$

$$\left. \begin{aligned} h(x_1, x_2, \xi, t) &= \xi(x_1, x_2, t) \\ \underline{K} \nabla h \cdot \vec{n} &= (I - S_y \frac{\partial \xi}{\partial t}) \end{aligned} \right\} \quad \text{on } \Gamma_4 \text{ (Free surface)} \quad (36)$$

$$\left. \begin{aligned} |\underline{K} \nabla h \cdot \vec{n}| &< E + E^* \\ \psi &> \psi_w \end{aligned} \right\} \quad \text{on } \Gamma_5 \text{ (Atmospheric boundary)} \quad (37)$$

$$-K_3 \nabla h \cdot \vec{n}_3 < K_3^s \quad \text{on } \Gamma_6 \text{ (Infiltration boundary)} \quad (38)$$

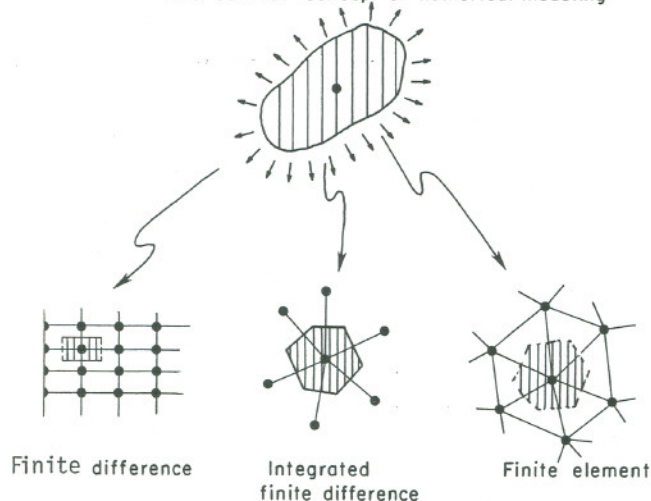
NUMERICAL METHODS OF MODELING

Formulation of Numerical Equations

As pointed out above, the governing equations of groundwater motion (29) and (31) are equations of mass conservation. The basic aim of numerical methods is to discretize the flow region into appropriately small subdomains, and to apply the mass conservation equation to each subdomain. For maximum accuracy, these subdomains must be sufficiently small so that the material properties and fluid potential do not vary significantly over each area of interest.

One such arbitrarily small subdomain is shown in Fig. 2a. Several techniques are available to define the shape and size of this subdomain and its relation to the flow region. In the classical finite difference method (Fig. 2b), which directly discretizes and approximates the partial differential equation (31), the subdomain of interest is implicitly defined by bounding surfaces normal to the coordinate axes and located midway between the nodal points.

The central concept of numerical modeling



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Fig. 2. The central theme of mathematical modeling.

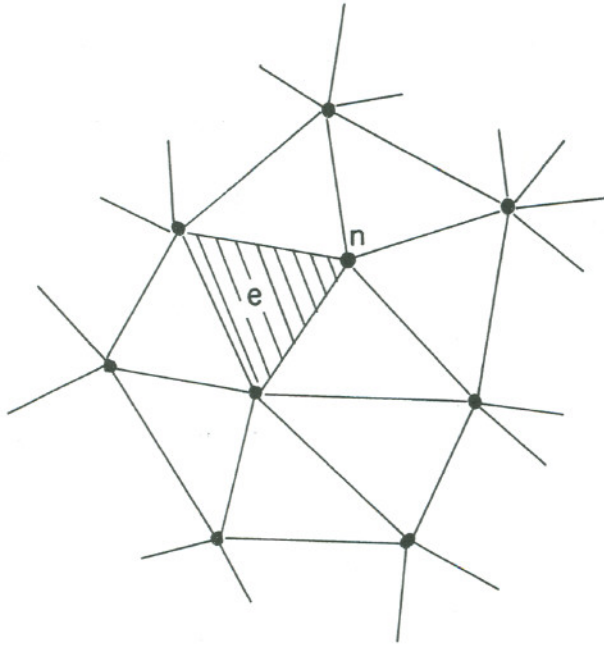
An alternative method is the integral approach (Figs. 2c, 2d), in which the rate of accumulation of mass within each subdomain is directly evaluated in order to implement mass conservation. The difference between the finite difference approach and the integral approach is a matter of detail in that the former treats the problem of mass conservation as one of equivalent velocity gradients, assuming linear velocity variations within the subdomain. In the integral approach, one may define the subdomain explicitly as in Fig. 2c so that the boundaries of the subdomain are defined *a priori*. Or, one can define the subdomain as a weighted fraction of a larger domain as in Fig. 2d, thereby implicitly defining the subdomain of interest. As we shall see, each of these approaches provides certain special advantages in achieving the same goal.

The closeness of the finite difference method (FDM) to the classical differential equation and the extensive mathematical literature associated with the latter, made FDM the natural choice in early numerical modeling work. However, the method is inherently tied to an orthogonal grid of nodal points, which makes it inconvenient in treating flow regions with complex geometrical shapes.

The need for improving the ability to handle problems of complex geometry has led many workers to integral formulations. The development of the integral approach has mainly followed two different lines. Workers in the field of heat transfer (Dusinberre, 1961; Edwards, 1969, 1972) and others in the field of groundwater (Tyson and Weber, 1964; Cooley, 1971) have restricted themselves to isotropic materials and extended the FDM in a simple fashion to what has since been termed the Integrated Finite Difference Method (IFDM) (Narasimhan and Witherspoon, 1976a). The governing equation in the IFDM is identical with (29) and can be obtained by integrating (31) in the space domain. In order to solve the equation numerically, the flow region is discretized into subdomains whose boundary surfaces are explicitly defined *a priori*. The nodal points within each subdomain are locations at which the average properties of the subdomains are represented. In the IFDM, nodal locations are so chosen that the lines joining adjacent nodal points are normal to the intervening interfaces (Fig. 2c). This makes it easy to define the normal gradient at the interface by simple finite differences and (29) can be directly solved by evaluating the surface intervals over each subdomain. The advantage of this simple and elegant approach is that it can easily handle problems with complex geometry. In addition, the approach is intrinsically multidimensional. The chief drawback, however, is that the discretization is designed only to evaluate normal gradients and hence the tangential gradients at interfaces cannot be readily evaluated. As a result, this method is unsuitable for handling materials with arbitrary anisotropy or with tensorial fields such as stress or dispersion, which require the evaluation of normal as well as tangential gradients at element boundaries. Moreover, the finite difference gradient approximation used in this approach cannot accurately approximate rapid changes in gradient unless the grid points are spaced very closely.

During the mid-1960s, structural engineers devoted much of their time to the development of an integral method which, unlike the IFDM, would be capable of handling general tensorial properties with great facility, in addition to handling complex geometry. Their efforts led to the development of an integral method which is now widely known as the Finite Element Method (FEM). As can be seen from Figs. 2c and 2d, one of the differences between the IFDM and FEM is that in the former the subdomain is explicitly defined and in the latter, it is a weighted fraction of a larger domain made up of triangles.

Although the early FEM equations were developed from physical considerations (Winslow, 1966; Wilson, 1968), later workers have developed FEM equations using a variety of mathematical techniques such as variational principles (Javandel and Witherspoon, 1968), the Galerkin Method (Zienkiewicz and Parekh, 1970; Pinder and Frind, 1972; Neuman, 1973b) or by the Method of Weighted Residuals (Finlayson, 1972). It was pointed out by Finlayson and Scriven (1967) that from a computational viewpoint the Galerkin approach forms the most direct method of formulating the FEM equations. The Galerkin procedure, which is a type of the weighted residual method, essentially consists of the following.



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Fig. 3. Discretization of flow region into a system of finite elements, e.

The flow region is first discretized into a system of triangles as in Fig. 3. More general shapes such as quadrilaterals can be used with equal ease, and we are considering triangles only for simplicity. Within the flow region let the dependent variable h vary by the linear relation

$$h \approx h' = \xi_m(x_i)h_m(t), \quad \begin{matrix} m = 1, 2, 3, \dots, N \\ i = 1, 2, 3 \end{matrix} \quad (39)$$

where the repetition of the subscript m implies summation. The function $\xi_m(x_i)$ is called a basis function, defined in such a way that $\xi_m(x_i) = 1$ at nodal point m and zero at all other nodal points. The quantities $h_m(t)$ are undetermined coefficients. In the case of the triangular elements of Fig. 3, ξ_m varies linearly over all the elements which have m as a corner point. We now substitute (39) for ψ into (31), multiply the PDE by the weighting function ξ_n (the Galerkin weighting function) and integrate over the entire flow region to obtain (Pinder and Frind, 1972)

$$\sum_e \int_V \xi_n [\nabla \cdot \underline{K} \nabla \xi_m h_m - m_c \frac{\partial \xi_m h_m}{\partial t}] dV = 0 \quad (40)$$

$n = 1, 2, 3 \dots N.$

Equation 40 implies that there are N basis functions and it has been shown by Forray (1968) that $N \rightarrow \infty$, $h' \rightarrow h$. Next, Green's first identity (Sokolnikoff and Redheffer, 1966) is applied to (40) to eliminate the second derivative and (40) reduces to

$$\sum_e \left[\int_V \nabla \xi_n \cdot \underline{K} \nabla \xi_m h_m dV + \int_V m_c \xi_n \xi_m \frac{\partial h_m}{\partial t} dV - \int_{\Gamma^e} \xi_n \underline{K} \nabla \xi_m h_m \cdot \vec{n} d\Gamma \right] = 0 \quad (41)$$

The surface integral in (41) is nonzero only when the surface of integration coincides with the external surface of the flow region, and then it is prescribed and known. The task of the FEM is therefore to evaluate the two volume integrals in (41).

Although the general form of the Galerkin formulation is well established, some workers (e.g. Neuman, 1973b) have found that the substitution of $h' \approx \xi_m h_m$ into the time derivative in (40), which gives rise to the so-called consistent mass matrix (Fujii, 1973), may lead to difficulties of convergence or oscillatory solutions. Fujii (1973) has shown on theoretical grounds that under certain conditions, the numerical solution of (41) can violate the Maximum Principle, which states that in the absence of sources or sinks, the maximum potential can occur at the initial time or on the boundary. Narasimhan (1976) found that the numerical solution of (41) may not assure local mass balance although global mass balance may still be preserved. For these reasons, Neuman and Narasimhan (1976) restrict the application of the approximation (39) strictly to the space domain (which gives rise to the so-called lumped mass matrix) and write

$$\sum_c \left[\int_V \nabla \xi_n \cdot \underline{K} \nabla \xi_m h_m dV + \int_V m_c \xi_n \frac{\partial h_m}{\partial t} dV - \int_{\Gamma^e} \xi_n \underline{K} \nabla \xi_m h_m \cdot \vec{n} d\Gamma \right] = 0 \quad (42)$$

in which $\bar{h}^N$ is the mean value of potential over the subdomain associated with nodal point n .

At this point it is appropriate to outline some of the special advantages of the FEM. By introducing a surface $h = \xi_m h_m$ for the variation of potential over an elemental region, the FEM achieves a general and powerful method of evaluating gradients, which results in three important advantages: (a) it is very convenient in handling arbitrary tensorial quantities such as stress, anisotropy, and dispersion; (b) it is possible to fit higher-order surfaces to the variation of potentials over an elemental region, thereby greatly enhancing the accuracy of evaluating spatial derivatives; and (c) it is possible to approximate complex geometries efficiently by appropriate choice of elemental blocks.

The concept of isoparametric elements is a powerful recent extension of the FEM (Zienkiewicz, 1971; Ergatoudis et al., 1968; Pinder and Frind, 1972). Note that the spatial function $\xi_n(x_i)$ is sufficiently general in nature as to admit of first, second or higher degree algebraic functions. Isoparametric elements are constructed by letting ξ_n be an appropriate higher-order form and making use of curvilinear coordinate transformations. The remarkable feature of the isoparametric elements is that the higher-order approximation not only defines the spatial variation of the dependent variable more accurately, but also enables the handling of curved geometries. In two dimensions, isoparametric elements are curvilinear quadrilaterals, while in three dimensions they may be curvilinear parallelipeds. Isoparametric elements may be quadratic or cubic, depending on whether ξ_n is of second or third degree. The nature of the isoparametric elements is such that a higher-order element need not necessarily be more accurate than a lower-order element (Emery and Carson, 1971). Superparametric and subparametric elements are sometimes used when the variation of potential and the boundary shapes of the elements are to be approximated to different orders of accuracy. Some workers, especially in the field of petroleum engineering, tend to use the power of (39) only for achieving a higher-order approximation for the spatial variation of potential and not for handling curvilinear boundaries. In this approach, the higher-order approximations are used in conjunction with an orthogonal, rectangular grid of mesh points.

It was mentioned earlier that the IFDM is based on surface integration, while the FEM is based on the evaluation of volume integrals. In the case of the simple triangular elements shown in Fig. 3, the equivalence between volume integration and surface integration can easily be recognized (Narasimhan, 1975), leading to an understanding of the conceptual similarities between the two schemes. When the higher-order isoparametric elements are employed, the FEM makes use of selected quadrature points within the element at which the integrals are numerically evaluated.

The Equation Matrices

In the previous section it was shown that the governing equations for the FDM and the IFDM are

given by (31) and (29), respectively. The FEM, on the other hand, lends itself to two forms: a consistent mass matrix form (44) as well as a lumped mass matrix form (43). Of these, (31), (29) and (42) all lead to a matrix (Type 1), while (41) leads to a nondiagonal fluid mass capacity matrix (Type 2). These two systems of equations may be written:

$$\text{Type 1} \quad [A]\{h\} + [D^*]\{\dot{h}\} = \{Q\} \quad (43)$$

$$\text{Type 2} \quad [A]\{h\} + [D]\{\dot{h}\} = \{Q\} \quad (44)$$

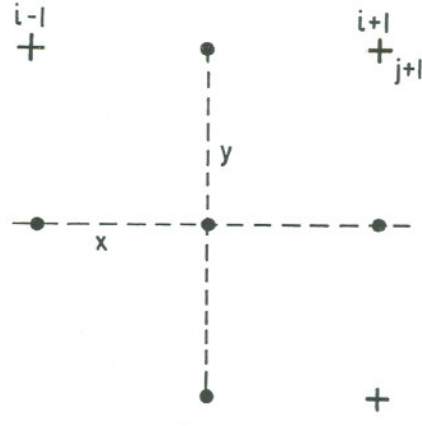
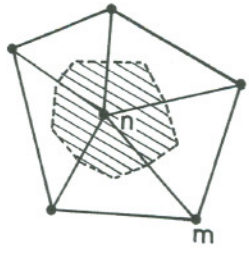
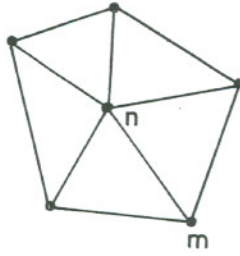
Each row in the above systems of equations represents the evaluation of mass balance for one nodal point of interest in the system. The matrix $[A]$ is a conductance matrix (or "stiffness" matrix as it is often called), which summarizes the coefficients determining mass transfer between connected mass balance subdomains. It is a symmetric, sparse, and usually diagonal matrix. $[D^*]$ and $[D]$ are matrices of fluid mass capacity, with the asterisk in (43) denoting the fact that the nondiagonal terms in the matrix are zero and $\{Q\}$ is a vector of known source terms. An examination of (44) will also show that the mass balance equation for a given nodal point (a certain row in the system) also contains the time derivatives of the neighboring nodal points, while in (43) the evaluation of mass balance for a given nodal point contains only its own time derivative. As a consequence, (44) not only requires more computer storage but also involves more computational operations. Note that the various methods (FDM, IFDM, FEM) differ primarily in the techniques employed in assembling the various components of the matrices, and it is these techniques which endow the different methods with their special advantages for selected situations.

So far, the comparisons between the different methods have been made on conceptual grounds. In a recent work Wang and Anderson (1976) examined the algebraic equations for the Laplace equation derived for FDM and FEM and found that in several cases, the same set of algebraic equations are generated in more than one way and that the choice of the element shape and basis functions in the FEM is analogous to the choice of integration rule in the FDM.

Once the appropriate system of equations (43) or (44) is chosen, the solution strategy is to choose an appropriate time interval Δt , solve for $\{h\}$ using the known initial condition at t_0 , advance to the next time level $t_0 + \Delta t$, and repeat the process once again. Note that since h changes continuously during Δt , it is necessary to use appropriate mean values of $\{h\} = \{h\}$ in the systems of equations before a solution can be attempted.

Substitution of $\{h\} = \{h^0\}$ (where the superscript 0 denotes the known initial values) in (43) leads to a set of equations in which all quantities are known except the unknown time derivatives $\{\dot{h}\}$, which can now be computed explicitly. These equations are summarized by Equations 1, 2, and 3 in Table I. On the other hand, no such explicit computations are possible in the case of (44) in which the time derivatives of neighboring nodes are part of the mass balance equation for a given

Table I. Summary of Numerical Equations

	<u>Explicit Formulations</u>
Equation (1) FDM $G_{i,j} + \frac{1}{(\Delta x)^2} [\bar{K}_{i-1,j} (h_{i-1,j}^{\circ} - h_{i,j}^{\circ}) + \bar{K}_{i,j} (h_{i+1,j}^{\circ} - h_{i,j}^{\circ}) + \frac{1}{(\Delta y)^2} [\bar{K}_{i,j-1} (h_{i,j-1}^{\circ} - h_{i,j}^{\circ}) + \bar{K}_{i,j} (h_{i,j+1}^{\circ} - h_{i,j}^{\circ})]$ $= m_{c,i,j} \frac{\Delta h_{i,j}}{\Delta t}$	
(2) IFDM $V_n G_n + \sum_m \frac{\bar{K}_{n,m} A_{n,m}}{D_{n,m}} (h_m^{\circ} - h_n^{\circ})$ $= M_{c,n} \frac{\Delta h_n}{\Delta t}$	
(3) FEM $\sum_e \left\{ G_n \int_{V^e} \xi_n dV - \int_{V^e} \Delta \xi_n \cdot K \Delta \xi_m h_m dV \right\}$ $\left\{ \sum_e m_{c,e} \int_{V^e} \xi_n dV \right\} \frac{\Delta h_n}{\Delta t}$	
<u>Non-explicit Formulation</u> (Consistent Mass Matrix)	
(4) FEM $\sum_e \left\{ G_n \int_{V^e} \xi_n dV - \int_{V^e} \Delta \xi_n \cdot K \Delta \xi_m \cdot h_m dV \right\}$ $= \left\{ \sum_e m_{c,e} \int_{V^e} \xi_n \xi_n dV \right\} \frac{\Delta h_n}{\Delta t}$ $+ \left\{ \sum_e m_{c,e} \left[\int_{V^e} \xi_n \xi_m dV \right] \right\} \frac{\Delta h_m}{\Delta t}$	

node. Thus, (43) and (44) give rise to explicit and nonexplicit algebraic equations as shown in Table I. The explicit equation for a given node, in the light of (43), is

$$h_n = \frac{Q_n - \sum_m A_{nm} h_m}{D_{nn}^*} \quad (45)$$

Stability and Implicit Equation

The explicit equation 45 with its inherent simplicity is only of limited value since it is subject to severe time constraints. The solution obtained with (45) can oscillate violently and become unstable if the discrete time step Δt used in the calculations exceeds some critical value. As pointed out by Richtmeyer and Morton, (1967, p. 26), stability is a local problem restricted to the vicinity of the subdomain over which mass balance is being evaluated. Physically (Edwards, 1972; Narasimhan, 1975; Neuman and Narasimhan, 1976), the time limit critical to stability in the vicinity of a point n in the flow domain is governed by the fluid mass capacity of the subdomain associated with it ($M_{c,n}$ or D_{nn}^*) and the sum of the "surface conductances" represented by $-\sum_m A_{nm}$. Thus the time step critical to stability in the vicinity of point n is given by Narasimhan and Witherspoon, 1976a; Neuman and Narasimhan, 1976)

$$t_{stab,n} = \frac{D_{nn}^*}{-\sum_{m \neq n} A_{nm}} \quad (46)$$

Note that the criterion (46) is valid in three dimensions and is independent of coordinate systems.

Often it is necessary, on grounds of cost and effort, to use time steps much larger than $\Delta t_{stab,n}$. For such purposes, it is necessary to discard the explicit equations in favor of the implicit ones. The implicit equations are obtained by substituting in (43) or (44), $\{h\} = \{h^0 + \lambda \dot{h}\}$ $0 \leq \lambda \leq 1$. Note that $\lambda = 0, 0.5$, and 1 correspond to the explicit, central differencing, and backward differencing schemes, respectively. For unconditional stability, $0.5 \leq \lambda \leq 1.0$. The systems of implicit equations stemming from (43) and (44) are, respectively,

$$\text{Type I} \quad [\underline{A}]\{h + \lambda \dot{h}\} + [\underline{D}^*]\{\dot{h}\} = \{Q\}, \quad (47)$$

$$\text{Type II} \quad [\underline{A}]\{h + \lambda \dot{h}\} + [\underline{D}]\{\dot{h}\} = \{Q\}. \quad (48)$$

In contrast to the explicit equation, the only way to determine the unknown vector $\{\dot{h}\}$ in the case of the nonexplicit equation (44) as well as the implicit equations 47 and 48 is to solve the system of simultaneous equations by appropriate methods.

Solution Techniques

One of the major tasks of mathematical modeling is that of seeking an efficient process for solving the system of implicit, simultaneous equations (47) or (48) and compute $\{h\}$. The power of a given model may often be governed by the method

selected for solving the system of simultaneous equations. In general, two categories of techniques are available: direct methods and iterative methods (see for example, Scarborough, 1966). The direct method can further be subdivided into solution by determinants; solution by successive elimination of the unknowns; and solution by inversion of matrices. Perhaps the most widely used direct approach for transient problems is that of successive elimination and back substitution, which includes the Gaussian elimination method (Scarborough, 1966) and the Cholesky decomposition method (Weaver, 1967).

The direct methods of solving systems of simultaneous equations involve many subtractions of terms of the same order of magnitude. When such terms are nearly equal, their differences can be very small and the inaccuracies due to this inherent weakness of direct methods cannot be entirely avoided. Another difficulty inherent in the direct methods relates to the requirements of computer storage. The $[\underline{A}]$ and the $[\underline{D}]$ matrices occurring in (47) and (48) are both sparse in nature. In order to minimize the influence of sparseness on computer storage and computational effort, the matrices should be made to have as small a bandwidth as possible. One way to achieve this is to use an efficient scheme of numbering the mesh points (Pinder and Frind, 1972). Even with optimal nodal numbering, the bandwidth may prove to be unavoidably large in three-dimensional problems and may greatly increase the requirements for computer storage.

This has tended to discourage the extension of FEM algorithms to three-dimensional problems. A great deal of attention has therefore been spent in developing techniques to overcome this limitation of the FEM. One such technique is that of the frontal solution, which only requires an optimal number of elements. More recently, Gupta and Tanji (1976) resorted to the use of intermediate disk or tape storage to store and retrieve results that are repeatedly used. They solved a three-dimensional steady-state problem in this manner using the FEM.

One way to avoid the difficulties associated with the direct solution of large matrices is to develop iterative techniques. Extensive mathematical literature is available on iterative techniques (e.g. Southwell, 1946; Varga, 1962). The central concept of the iterative approach is to start with an assumed approximate solution and progressively refine the same. To speed up the process of refinement, artifacts such as relaxation or acceleration factors may be used.

The iteration methods are often free from the inaccuracies inherent in the direct solution schemes resulting from the subtraction of near-equal terms. The iterative schemes are self-correcting since the errors made during one iteration are corrected in the subsequent iterations. Also, iterative schemes avoid the need for storing large sparse matrices, and this makes them especially desirable in handling problems involving a large number of mesh points.

Numerous iterative schemes have been devel-

oped in the literature. Among these may be mentioned: The point Jacobi, Gauss-Seidel and Successive over-relaxation methods (Varga, 1962); the Alternating Direction Implicit Procedure (Douglas and Rachford, 1956); the Alternating Direction Implicit Iterative Technique (Wachpress and Habetler, 1960); the Strongly Implicit Procedure (Stone, 1968); and the accelerated mixed explicit-implicit scheme (Edwards, 1972; Narasimhan et al., 1976c).

Although many iterative methods are available, no one method is best suited for all problems. Since iterative methods start from an assumed approximate solution, the efficiency of iteration is dependent on the choice of the approximation, and this makes the iterative approach undesirable in solving steady-state problems as compared to direct methods.

To speed up the iteration process, relaxation and acceleration factors are often used. Unfortunately, these factors may often be problem dependent. Also, an important feature of the iterative approach is to decide *a priori*, an error tolerance limit to stop the iteration process. Such a limit may also be problem dependent.

Perhaps the greatest limitation of the iterative schemes is the requirement that the matrix be well conditioned. An ill-conditioned matrix may drastically affect the rate of convergence or even prevent convergence of the iterative scheme. Gambolati (1975c) demonstrated the importance of a diagonally dominant matrix in solving the FEM by iterative schemes. Neuman and Narasimhan (1976) have shown how diagonal dominance of the matrix can be achieved even in heterogeneous, anisotropic media by properly designing the discretized mesh.

The question as to which solution approach is to be preferred is difficult to answer. For steady-state problems (Poisson's equation, Laplace's equation), direct methods seem superior to iterative techniques. In the case of transient problems involving a large number of mesh points, the direct methods may prove to be less desirable than the iterative techniques due to increased computer-storage requirements and reduced speed of computation.

Some Special Aspects of Interest

Time Integration of Fluxes: An essential step in solving the transient groundwater flow equation is that of evaluating the magnitude of mass transfer during t between two interacting subdomains. The mass transfer M_{nm} into subdomain m from subdomain n is given by

$$M_{nm} = A_{nm} [h_n - h_m] \Delta t \quad (49)$$

Since h_n and h_m are both varying during Δt , we choose to approximately evaluate M_{nm} by using the mean values $h_n = h_n^o + \lambda \Delta h_n$ and $h_m = h_m^o + \lambda \Delta h_m$. The accuracy in the evaluation of M_{nm} is thus directly related to the accuracy of the chosen mean value, which, in turn, is governed by the selected value of λ . If Δt is small and h_n and h_m both vary linearly during Δt , then the correct M_{nm} can be estimated by choosing $\lambda = 0.5$ (central differencing or Crank-Nicolson scheme). However,

if h_n and h_m change nonlinearly during Δt , as is especially likely when Δt is large, the choice of $\lambda = 0.5$ would lead to an inaccurate estimate of M_{nm} . Some workers have directed their attention towards minimizing errors of this type.

Edwards (1972) (see also Narasimhan et al., 1976) seeks to improve accuracy in computing M_{nm} by making an appropriate choice of the weighting factor. Towards this end, the time derivatives of the maximum changes in potentials during the previous two time steps are stored in memory. Assuming an exponential decay for falling potentials or a quadratic variation for rising potentials, $0.5 \leq \lambda \leq 1$ is appropriately chosen so that a best estimate of M_{nm} is obtained. Thus, for small time steps or when time derivatives are not changing rapidly, λ is chosen close to 0.5. For large time steps of when the system is approaching steady state, the appropriate value of λ is closer to 1.0.

The accuracy of flux integration could also be effectively improved using the FEM. Oden (1969) discussed how this could be achieved by extending the FEM to the time domain. Thus, instead of using the approximation suggested in (39) one uses $\psi \approx \xi_m(x_i, t) \psi_m$. Zienkiewicz and Perekh (1970) proposed that the time-domain extension of the FEM could be used for transient field problems. Following this, Gray and Pinder (1974) have demonstrated the feasibility of using the new FEM technique. However, they conclude that the selection of an optimum numerical solution scheme to implement the new approach is dependent on the particular problem as well as the sequence of time steps used.

Handling of Heterogeneities and Anisotropy: Realistic groundwater problems are almost invariably characterized by spatial variability of material properties, i.e., heterogeneity and anisotropy.

In the finite-element method, integration of fluxes is performed element by element and each element is composed of a single material. If the material properties do not vary within the element, then the problem of heterogeneity is automatically taken care of in the element during integration. However, if a material property such as permeability were to vary spatially within the element, Pinder et al. (1973) describe a way of accounting for the variability using functional coefficients.

The nature of the FDM and the IFDM approaches (Figs. 2b and 2c) is such that mean values of material properties are associated at the representative nodal point locations, whereas the fluxes are evaluated at the interfaces between nodal points. Hence, appropriate mean values of permeability are to be used at the interfaces where the fluxes are evaluated. For this purpose it is often advantageous to use a harmonic mean permeability (Edwards, 1972; Narasimhan, 1975) which assures continuity of flux at the interface.

In an anisotropic medium, computation of flux across an arbitrary surface requires information on the hydraulic gradients normal to the surface

as well as the tangential hydraulic gradient along the surface. The effect of the tangential gradient, however, vanishes when the surface is normal to a principal axis of anisotropy. The FDM and the IFDM, which evaluate only the gradients normal to a surface of interest, are therefore inherently incapable of handling cases in which the principal axes of anisotropy are arbitrarily oriented in relation to the grid orientation. These two methods can handle anisotropy only when the grid lines coincide with the principal axes of anisotropy.

The FEM, on the other hand, because of its generalized representation of potential variation in space, can handle anisotropy in the most general terms. Thus, in the FEM the mesh orientation can be arbitrary in relation to the orientation of the axes of anisotropy. Nevertheless, in order to account for arbitrary anisotropy, it is necessary to compute the nondiagonal terms of the hydraulic conductivity matrix and this leads to increased computations in setting up the $[A]$ matrix. In nonlinear problems when the $[A]$ matrix has to be generated for every time step, calculation of the nondiagonal terms of the hydraulic conductivity matrix may prove to be costly. For this reason, many workers using the FEM would prefer orienting the FEM mesh parallel to the principal axes of anisotropy, whenever possible.

Nonlinear Coefficients: Many groundwater problems of interest involve the variation of K as well as m_c as a function of time or the hydraulic head. Perhaps the easiest method of accounting for these nonlinearities is to treat the nonlinear equation as a quasilinear equation with K and m_c treated as step functions in time. For a given time step, these values may be set equal to their values at the initial time step or may be estimated at the end of the time step $t + \Delta t$, or at the mean position, $t + \lambda \Delta t$. The quasilinearization approach may lead to significant mass-balance errors when both K and m_c vary rapidly with t or h or when Δt is very large. To avoid these mass balance errors, it may be necessary to limit the choice of Δt so that the variation of K and m_c from one time step to the next is kept very small (Edwards, 1972). An alternate approach in handling nonlinear coefficients is to use an iterative scheme in which the coefficients are continually updated until appropriate mass balance is obtained.

Choice of Δt : An appropriate choice of time steps is of considerable practical interest in efficiently solving a given problem. Perhaps the best scheme is one in which the size of Δt is progressively increased with advancing time. Such progressive adjustments to Δt may be either based on arbitrary criteria or may be based on some criteria related to the system behavior. While these adjustments can be relatively easy to make in linear problems with smooth boundary conditions, difficulties may arise in strongly nonlinear problems with time-dependent boundary conditions. In such problems, arbitrary increases in Δt may give rise to accumulation of mass-balance errors with time, which in turn may lead to progressively deteriorating solutions. One method of minimizing such errors is to cut down and repeat time-step calculations at the onset of significant mass-

balance errors (Edwards, 1972). Another approach is to use the so-called Predictor-Corrector schemes in which the time step is reduced if the computed values and predicted behavior do not agree with each other within acceptable limits.

Reliability of the Solution: Because of the complexity of their geometry, boundary and initial conditions, and the variability of the coefficients in space and time, most groundwater problems are too difficult, if not impossible, to solve by analytical techniques. However, these problems can be solved numerically to obtain approximate solutions, but there is usually no rigorous criteria available either to say that the solution is the correct one or if it is unique. Probably the best that can be done under the circumstances is to make calculations on several mesh sizes with the assumption that when the solution does not further change as the mesh size is decreased, the solution is that of the governing differential equation for the same phenomena. Hence many solutions are accepted because they have "converged" and because they "look good" judging by the known physical results.

Control of Accuracy: The very nature of numerical models is that they can provide only approximate solutions. The solutions are subject to different sources of error and a proper appreciation of these error sources is essential for a judicious use of numerical models. The following discussion on the sources of error is based on Edwards (1972).

Six principal types of errors affect accuracy. These are:

- Modeling errors, arising from inaccurate material properties, inaccurate initial and boundary conditions, and interpolation errors in evaluating tabulated properties.
- Spatial truncation errors, arising from the subdivision of the system into discrete volume elements, for which average values of spatially dependent variables must be estimated.
- Time truncation errors, arising from the use of discrete time steps, for which average values of time-dependent variables must be estimated.
- Potential truncation errors, arising from the discrete changes in potential that occur at each node in each time step, for which average values of potential-dependent variables must be estimated.
- Convergence errors, arising from the use of iterative methods with arbitrary convergence criteria.
- Arithmetic truncation errors, arising from the accumulation of roundoff errors and from the loss of significant figures that result when numerical values of widely differing magnitude are added to each other or numerical values of similar magnitude are subtracted from each other.

Modeling errors can usually be estimated by

comparing the results obtained from using different models of the same system (e.g. Gilham and Farvolden, 1974). An alternate approach to estimating modeling errors is to make use of "sensitivity theory," in which the uncertainty inherent in material properties is taken into account during the calculational process and the computed results are accompanied by confidence limits. Yet another way to approach the problem is to treat the governing differential equation as a stochastic differential equation. Both the sensitivity-theory approach and the stochastic differential-equation approach are still in their infancy as far as groundwater modeling is concerned.

In systems using the first-degree approximation for approximating gradients (e.g. the finite-difference approximation), spatial-truncation errors are controlled by subdividing the system just finely enough so that nonlinear potential distributions are fitted within required accuracy by linear interpolation. Just how fine this should be in different parts of the system may be difficult to estimate in advance. Often a simplified version of the problem may be first solved to help in estimating the degree of subdivision in different parts of the system.

A more powerful way to control spatial-truncation error is to employ higher-order approximations to the spatial variation of potential, as is done in the case of the finite-element method or by using the nine-point finite-difference approximation (Yanosik and McCracken, 1976).

Time-truncation errors can be controlled either by limiting the maximum variation of potential during time step (e.g. Edwards, 1972) or by using higher-order approximations for the variation of potential in each time step (e.g. Gray and Pinder, 1974). It may be pointed out here that little can be gained by attempting to minimize time-truncation errors while spatial-truncation errors are allowed to accumulate.

When using quasilinear approximation for material properties dependent on the potential, potential-truncation errors can be controlled by limiting the maximum variation of potential during each time step so that the material properties do not change widely from one step to the next.

Convergence errors and rate of convergence of iterative schemes can be controlled with the help of the error-tolerance factor and the choice of relaxation (or acceleration) factors. Both these factors are problem dependent and are difficult to estimate in advance. In heterogeneous problems, convergence may be affected when thin elements with material of very high permeability are in contact with elements with material of low permeability. One way to avoid the difficulty is to lump several thin elements into one large element.

Arithmetic-truncation errors arising from accumulated roundoff errors are generally unimportant in comparison with modeling errors and space-, time- or potential-truncation errors. Truncation errors arising from algebraic addition of terms that are nearly equal but have opposite signs or that have widely different orders of magnitude,

can be quite serious. This is one reason why it is necessary to avoid very high conductances between intercommunicating mass-balance elements by lumping thin elements together.

Choice of a Method: A review of the many different mathematical tools that are available for modeling leads to the natural question as to the choice of the best method. Probably no one method is best for all problems. For any given class of problems the choice of the best possible method should take into consideration the number of features to be modeled and the details, the accuracy desired, and finally the effort that can be expended on the problem. Quite often the choice depends on a tradeoff among the various factors.

CASE HISTORIES

Toth (1962), who developed a theory of groundwater motion in small groundwater basins in Central Alberta, Canada, was among the earliest to attempt mathematical simulation of actual groundwater systems. Since then, such models have been used to simulate many regional groundwater systems around the world with varying degrees of complexity and success. To gain an idea of how successful these attempts have been, we will consider a few sample case histories from the literature, chosen primarily from American and Canadian investigators.

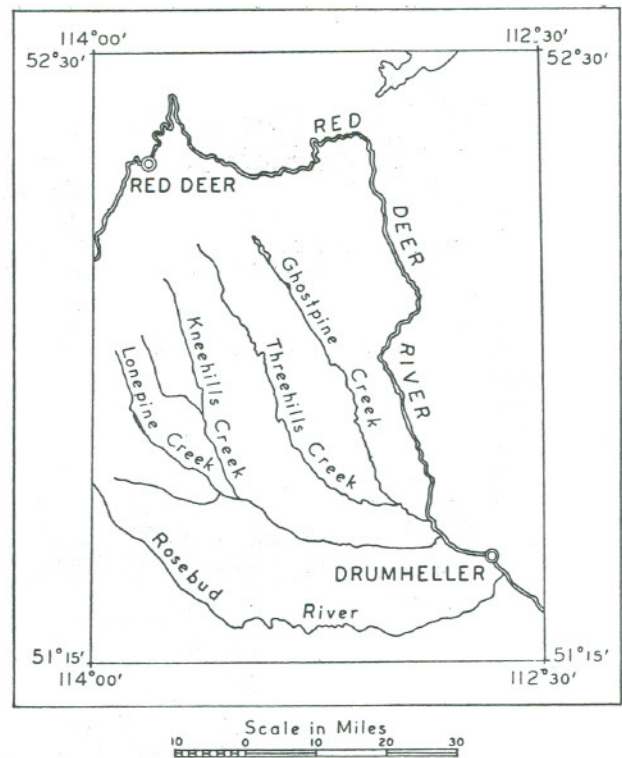
1. Toth (1962) Steady Groundwater Flow in Groundwater Basins in Central Alberta, Canada
2. Freeze and Witherspoon (1968) Steady Groundwater Flow in the Gravelbourg Aquifer, Saskatchewan, Canada
3. Pinder and Bredehoeft (1968) Dynamic Simulation of a Confined Aquifer at Musquodoboit Harbor, Nova Scotia, Canada
4. Prickett and Lonnquist (1971) Dynamic Simulation of the Cambrian-Ordovician Aquifer of Northeastern Illinois
5. Stephenson and Freeze (1974) Dynamic Simulation of Subsurface Flow -- Surface Water Run Off Relationship in the Reynolds Creek Watershed, Idaho
6. Feddes, et al. (1975) Dynamic Simulation of Unsaturated Flow and Plant Root Interaction in an Experimental Irrigation Field in De Groeve in Netherlands
7. Helm (1974) Dynamic, One-Dimensional Simulation of Land Subsidence at Pixley, California, Caused by Long Term Water Level Fluctuations
8. Gambolati et al. (1974) Dynamic Simulation of Land Subsidence at Venice, Italy
9. Lippmann (1973) Stochastic Simulation of the Mocho Subbasin of Livermore Valley, California

10. Emsellem and deMarsily (1971) Inverse Modeling of Alluvial Aquifer North of Strasbourg, France

On the basis of the parallel pattern of water divides and valleys in parts of Central Alberta (Fig. 4), and on the basis of inferred differences in permeability contrasts between geologic formations of the area, Toth (1962) considered individual, small drainage basins to be separate units of the groundwater flow regime. If one assumes that the phreatic surface is fixed and known, then the distribution of hydraulic head in the basin can be found by solving the Laplace equation under appropriate boundary conditions. Using the technique of separation of variables, Toth generated the two-dimensional profile shown in Fig. 5 that shows the division of flow across two adjacent valley sides. Simulations such as these helped Toth to recognize that in a typical groundwater basin one could mathematically distinguish between recharge areas (regions of predominantly downward groundwater motion) and discharge areas (regions of predominantly upward groundwater motion), separated by a median line. He also demonstrated how an uneven physiography or heterogeneity of material properties could lead to subgroundwater systems on different scales (local, intermediate, and regional) in a single groundwater basin.

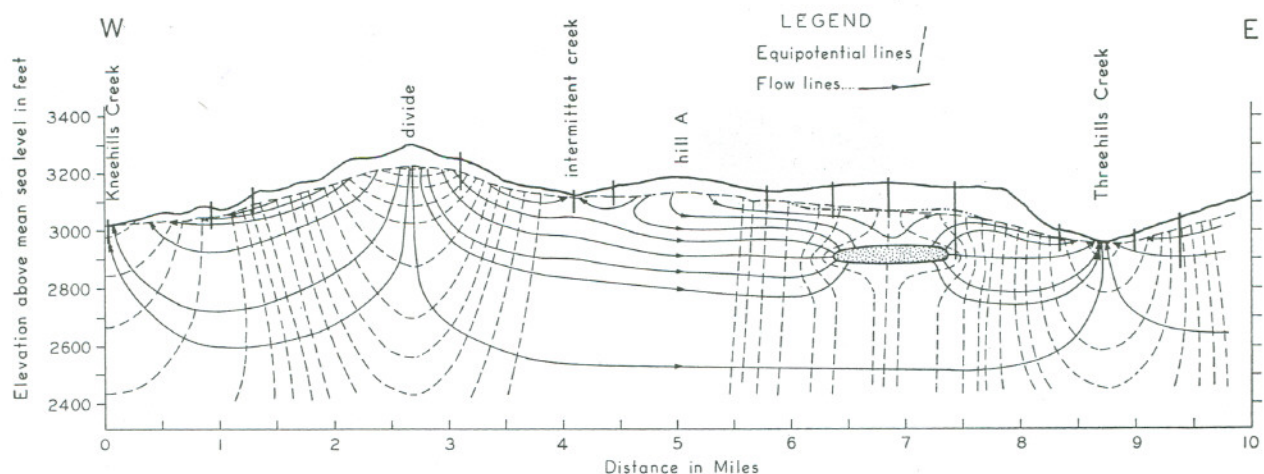
Perhaps the most important contribution of Toth's investigation was that it provided a formal framework for defining a groundwater basin and its anatomy. Such a framework is of vital interest not only in studying the movement of groundwater but also in interpreting the evolution of the geochemistry of groundwater (Chebotarev, 1955; Davis et al., 1959; Back, 1966).

Freeze and Witherspoon (1968) chose to use the finite difference approach of solving the Laplace equation and were thereby able to simulate far more complex basins than those simulated by Toth. In validating their numerical model, Freeze and Witherspoon modeled the two-dimensional steady-state flow pattern in the Gravelbourg aquifer, Saskatchewan, Canada, the hydrogeology of which had been extensively studied earlier. The results of their simulation are shown in Fig. 6. Their model not only considered the permeability contrasts between various units but also took into account a 20-to-1 anisotropy in certain layers. As can be seen from Fig. 6, the model was successful in simulating the hydrodynamics of the natural system with reasonable accuracy and effort. In an earlier work Freeze (1967) applied the finite-difference approach to simulate a three-dimensional field example as shown in Fig. 7.



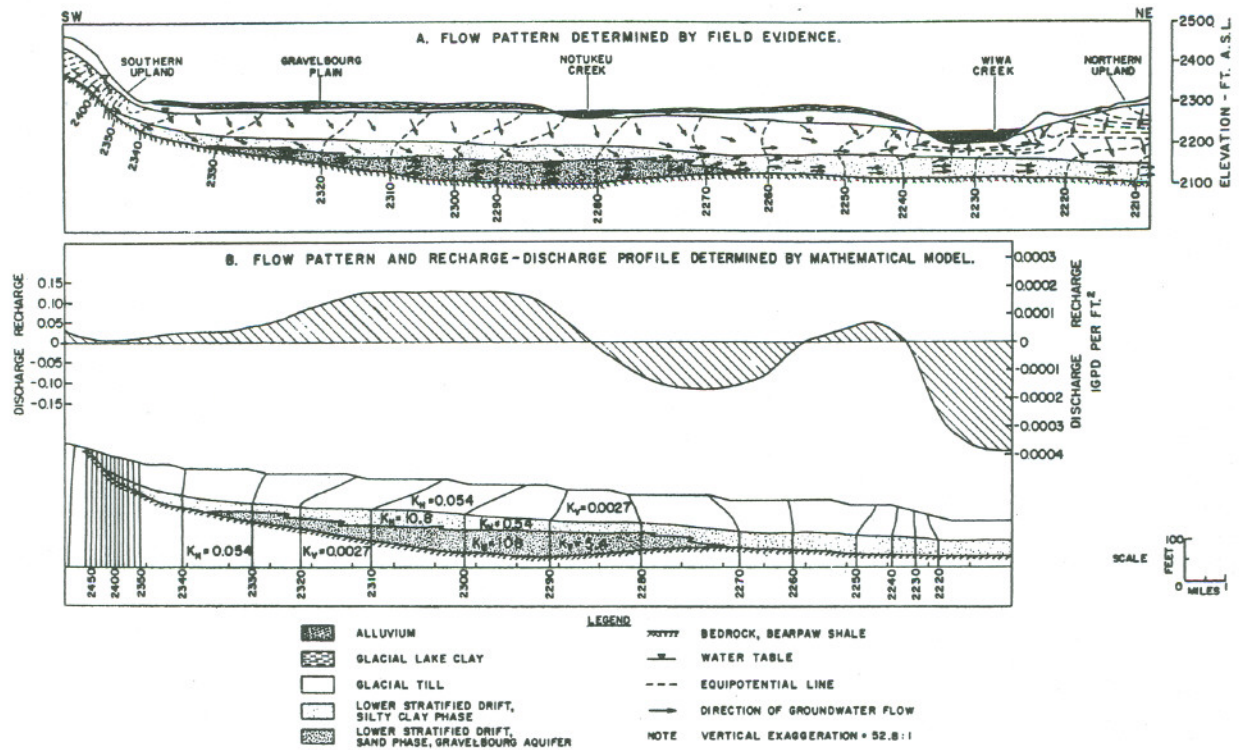
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Fig. 4. Parallelism of creeks in Central Alberta (Toth, 1962).



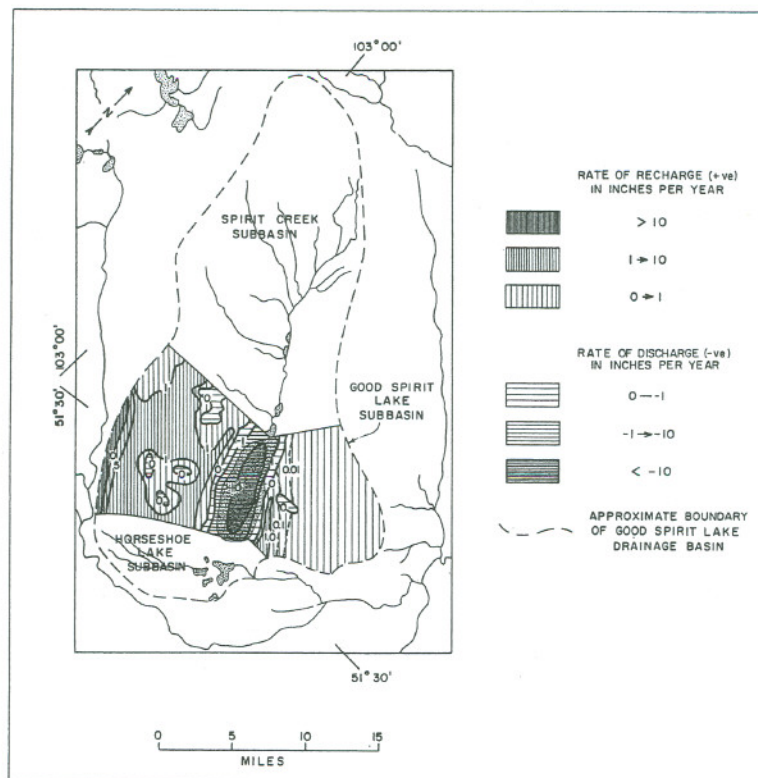
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Fig. 5. Steady-state flow pattern, a local flow system, and the effect of a highly permeable body across two adjacent valley sides in Central Alberta, Canada (Toth, 1962).



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Fig. 6. Steady-state flow pattern in the Gravelbourg aquifer, Saskatchewan, Canada: comparison of mathematical model with field data (Freeze and Witherspoon, 1968).



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Fig. 7. A recharge-discharge map from a three-dimensional field example, Good Spirit Lake drainage basin, Saskatchewan, Canada (Freeze and Witherspoon, 1968).

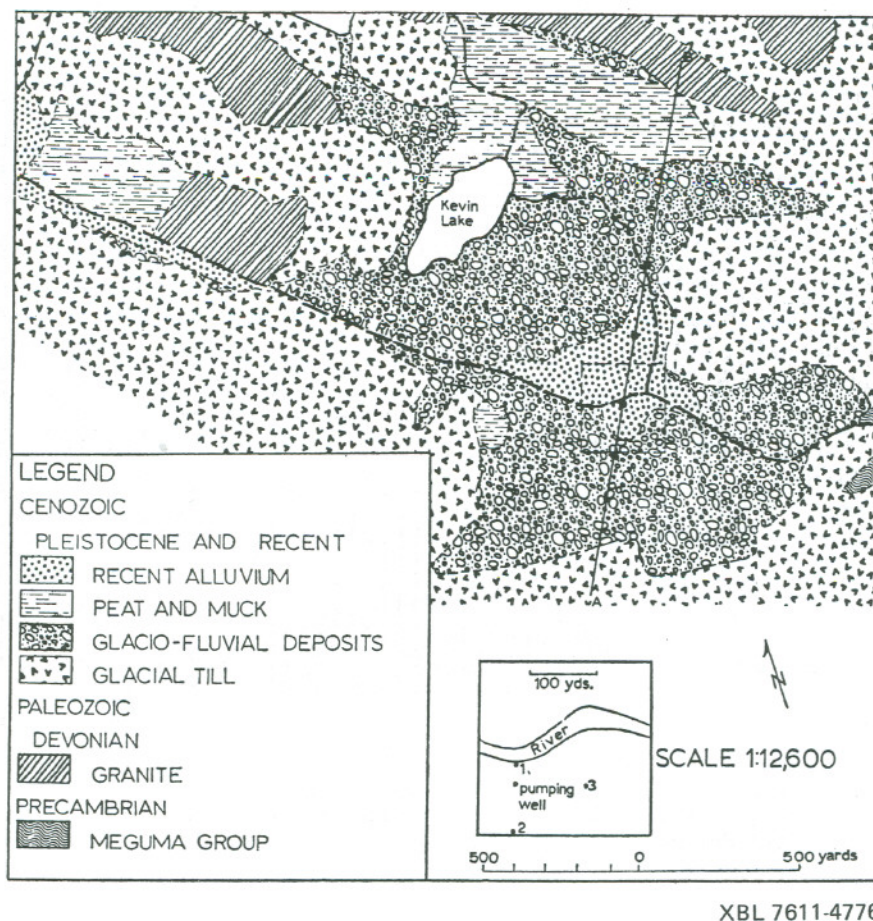


Fig. 8. Geologic map of Musquodoboit Harbour area, Nova Scotia, Canada (Pinder and Bredehoeft, 1968).

While Freeze and Witherspoon (1968) restricted their analysis to the steady-state situation, Pinder and Bredehoeft (1968) developed an implicit finite-difference model for simulating the dynamics of flow in a groundwater basin. They applied their model in evaluating the adequacy of an aquifer at the village of Musquodoboit Harbour, Nova Scotia, Canada (Fig. 8) as a source of water supply. As a first step in their investigation, Pinder and Bredehoeft had to estimate the distribution of aquifer parameters. To this end, they progressively modified the distribution of the parameters in the digital model until the model accurately simulated known pump-test data. Using the modified transmissibility matrix (Fig. 9), they went on to simulate the effects of a production well continuously producing at a rate of 0.963 cfs. (Fig. 10). The simulation led them to conclude that the aquifer would provide an adequate water supply to the village of Musquodoboit. As a check on the digital model, an electrical analog of the aquifer was also constructed and favorable comparisons were obtained between the two models.

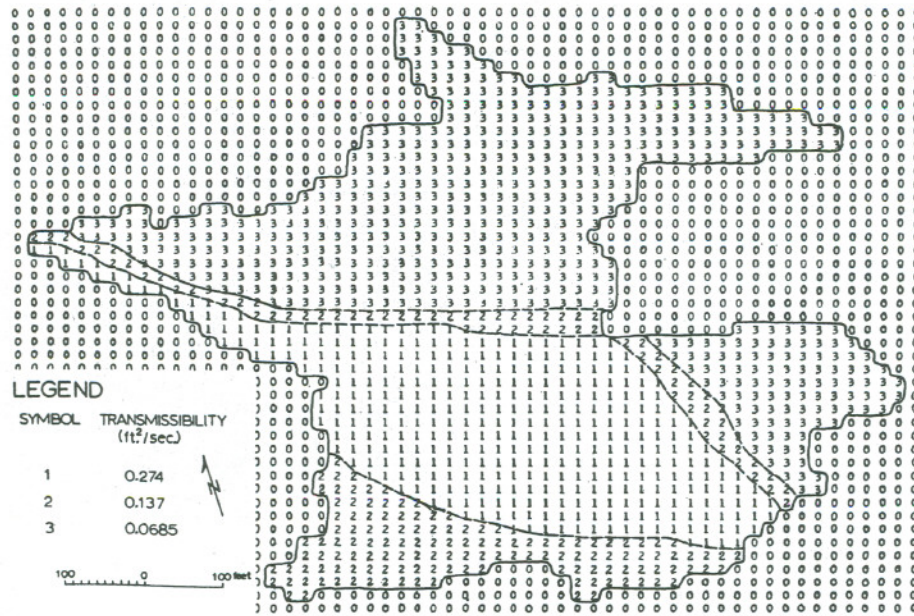
Prickett and Lonnquist (1971) applied the finite-difference technique to model the Cambrian-Ordovician aquifer in northeastern Illinois. This case history is of considerable interest in that the spatial as well as the temporal scales chosen for modeling are very large. The model was used

to simulate an area of approximately 24,000 square miles over a time period of 130 years.

The Cambrian-Ordovician aquifer, which is about 1000 ft thick, can be vertically divided into 4 hydraulically connected subunits, with the transmissivity decreasing from about 17,000 gdp/ft towards the top to almost zero towards the bottom (Fig. 11). The aquifer is under leaky artesian conditions and, in the northern parts of the simulated area, receives small quantities of recharge from the younger Silurian rocks or glacial drift through intervening shale formations of relatively low permeability.

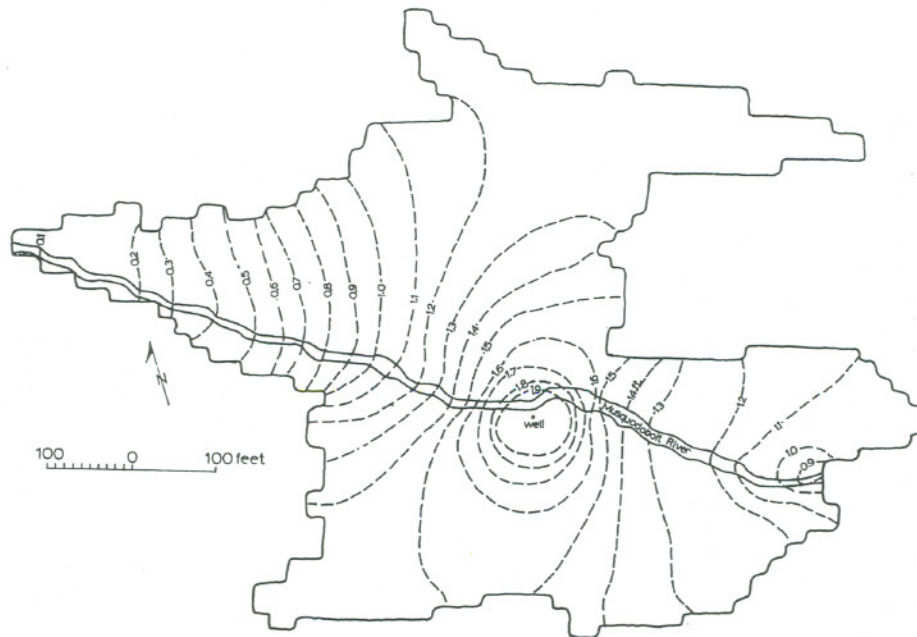
The Cambrian-Ordovician aquifer has been under intensive development since 1864 and the withdrawal has increased from about 200,000 gpd in 1864 to about 52,4 million gpd in 1960. Due to heavy pumpage, the piezometric surface had declined by as much as 600 ft in some parts of northeastern Illinois (Fig. 12). This excessive draw-down in the piezometric head has now converted the artesian aquifer to water-table conditions in some parts of the Chicago region.

The purpose of the Prickett-Lonnquist model was to predict the response of the Cambrian-Ordovician aquifer over a 130-year period from 1864-1995, using projected pumpage estimates in-



XBL 7611-4769

Fig. 9. Modified transmissibility matrix of the Musquodoboit aquifer adjusted on the basis of test-well logs and numerical simulation (Pinder and Bredehoeft, 1968).



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Fig. 10. Piezometric surface after 206.65 days of pumping at 0.963 cfs, as determined by the numerical model (Pinder and Bredehoeft, 1968).

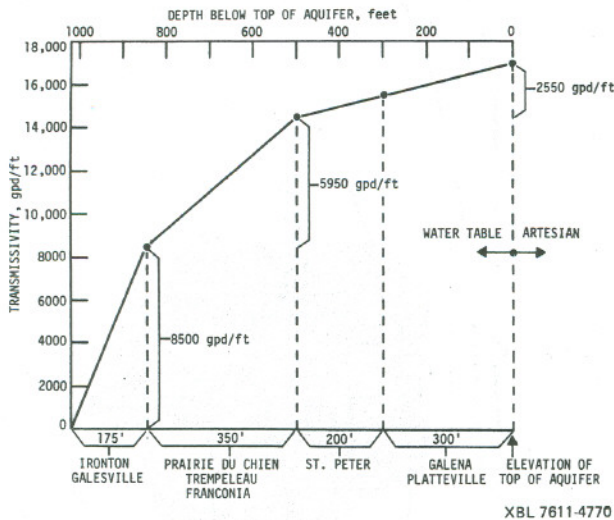
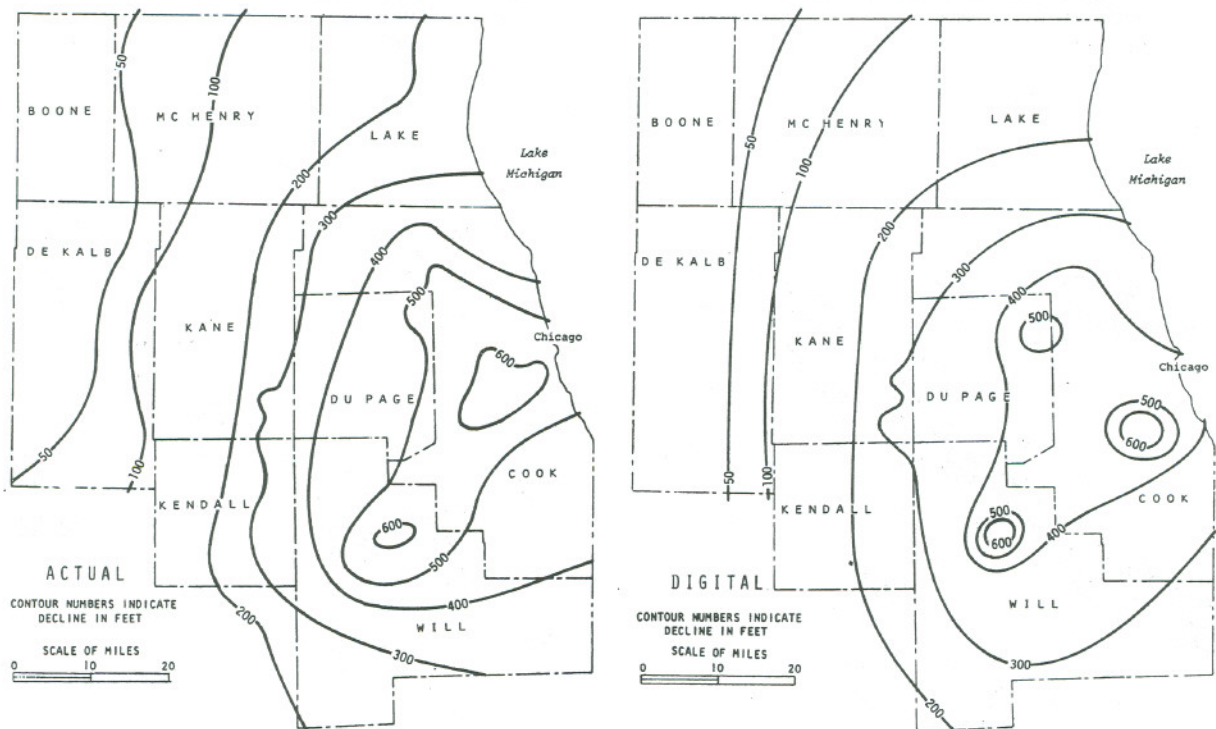


Fig. 11. Transmissivity variation of units of Cambrian-Ordovician aquifer in Chicago region (Prickett and Lonnquist, 1971).

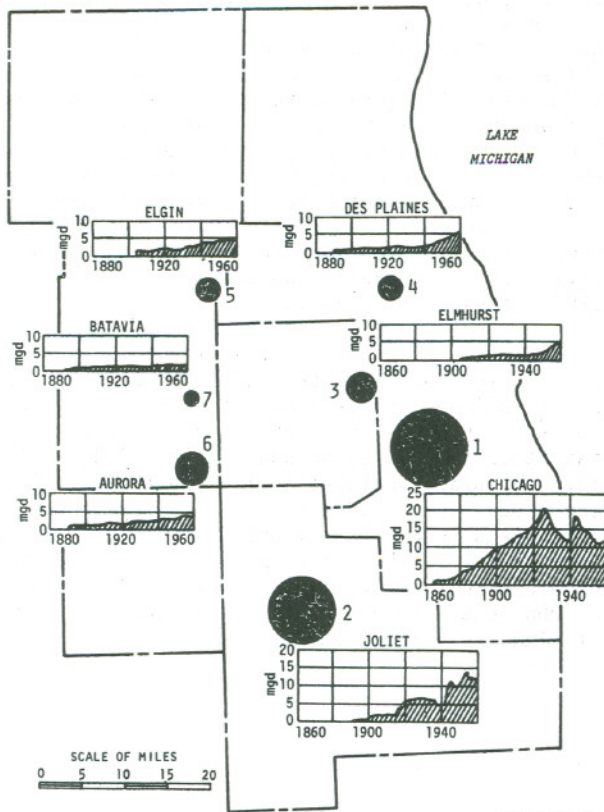
creasing to 145 million gpd in 1995. This model is a nonlinear model in that one can simulate a prescribed variation of pumpage with time (Fig. 13) as well as the decrease in transmissivity as a function of saturated thickness, when the aquifer undergoes dewatering. The artesian coefficient of storage was estimated to be 5×10^{-4} , while a specific storage of $5 \times 10^{-2} \text{ ft}^{-1}$ was used for the dewatering aquifer. Reasonable agreement between the model and the observed data for the period 1864-1958 can be seen in Fig. 12. The computed total declines in water level at the end of 1995 are shown in Fig. 14.

The interaction of the shallow groundwater system with surface water bodies through the unsaturated zone is often of interest to engineers concerned with water-balance studies related to watersheds. Stephenson and Freeze (1974) applied the unsaturated-saturated flow finite-difference model of Freeze (1971) to study runoff-generation mechanisms in an experimental watershed in Reynolds Creek, Idaho. Their aim was to simulate transient saturated-unsaturated flow contributions to stream discharge and to use the model as an aid in interpreting field measurements.



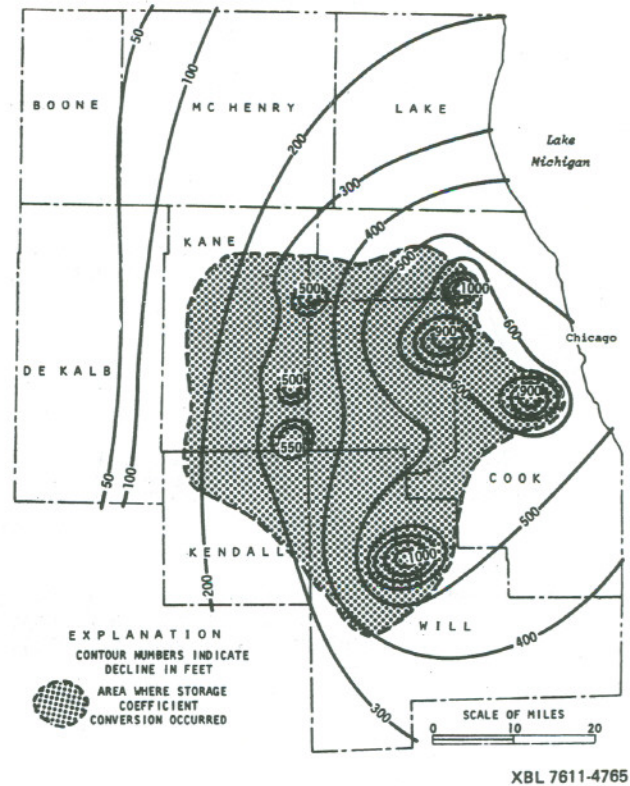
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Fig. 12. Piezometric declines in Cambrian-Ordovician aquifer, 1864-1958: comparison of field and numerical results (Prickett and Lonnquist, 1971).



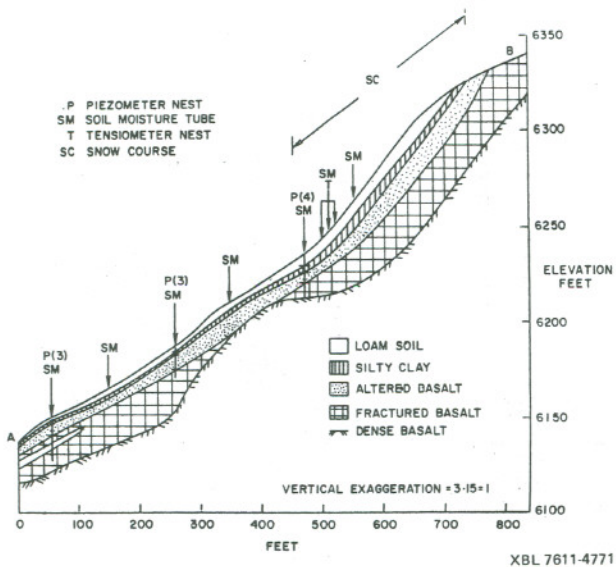
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Fig. 13. Pumpage history of the Cambrian-Ordovician aquifer (Prickett and Lonnquist, 1971).



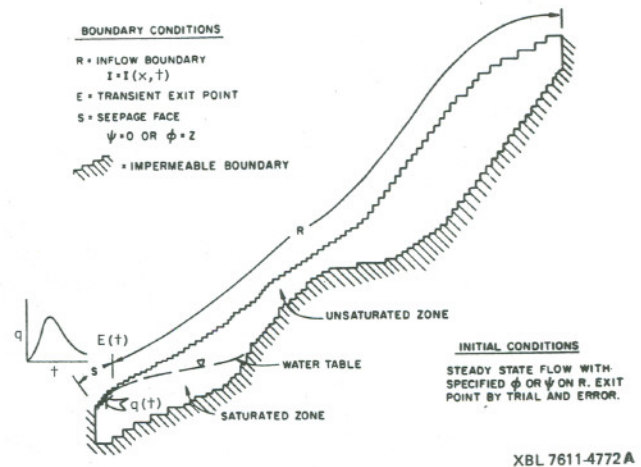
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Fig. 14. Computed piezometric declines, 1864-1995, in the Cambrian-Ordovician aquifer (Prickett and Lonnquist, 1971).



XBL 7611-4771

Fig. 15. Geologic cross section across Reynolds Creek, Idaho and guide to instrumentation (Stephenson and Freeze, 1974).



XBL 7611-4772A

Fig. 16. Boundary and initial conditions, simulation of Reynolds Creek, Idaho (Stephenson and Freeze, 1974).

The geologic profile at the site along with the disposition of field instrumentation is given in Fig. 15. The simulation problem was one of solving the parabolic nonlinear differential equation subject to the initial and boundary conditions shown in Fig. 16. The flow region contained

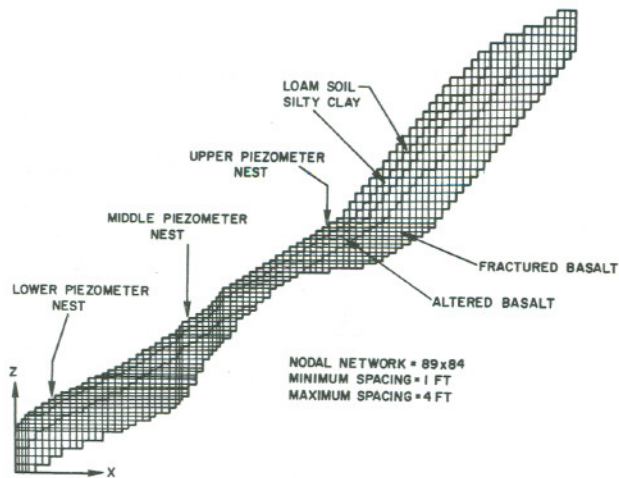


Fig. 17. Finite difference network for the Reynolds Creek basin, Idaho (Stephenson and Freeze, 1974).

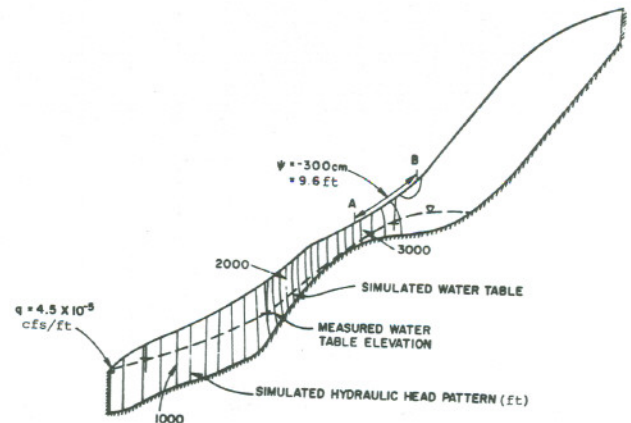


Fig. 18. Calibrated steady-state flow system for April 5, 1971, Reynolds Creek, Idaho (Stephenson and Freeze, 1974).

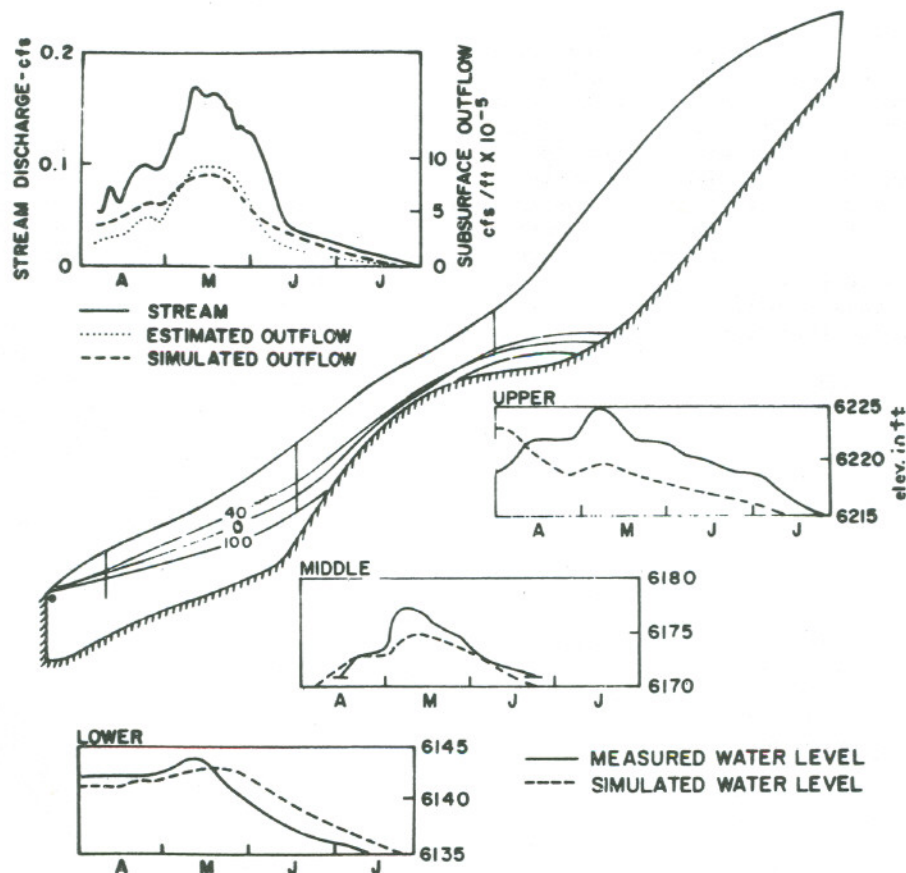


Fig. 19. Calibrated transient flow system for April 5 to July 13, 1971, Reynolds Creek, Idaho (Stephenson and Freeze, 1974).

three materials (fractured basalt, altered basalt, and soil) with saturated permeabilities varying from 3.8×10^{-4} to 15×10^{-4} dm/sec. K and varied with in the unsaturated zone, and soil compressibility was neglected due to its relative unimportance in near-surface systems. The finite-

difference network used in the simulation is shown in Fig. 17.

The primary task of Stephenson and Freeze was to calibrate the model by adjusting the input parameters and boundary conditions as well as the

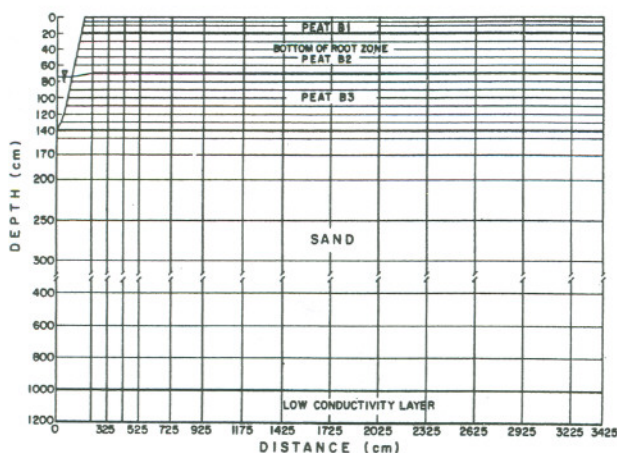
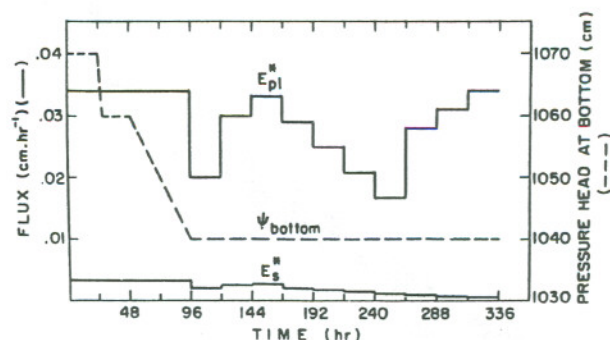


Fig. 20. Finite-element network of layered soil, De Groeve, Netherlands (Feddes et al., 1975).

geological configuration, using trial and error methods. The idea was to obtain a good fit with observed field data such as water table elevations, vertical hydraulic gradients at piezometer sites, the stream-flow hydrograph, pressure heads, and moisture contents. The calibrated steady-state system, which formed the initial conditions for the transient model, is shown in Fig. 18. The results of the transient simulation at the end of 100 days are presented in Fig. 19. This transient simulation was also effectively a calibration run, in that the saturated permeabilities of the three formations, as well as the inflow function over the inflow boundary, were adjusted to obtain the best match with field observations.

It can be seen in Fig. 19 that the calibrated model agrees reasonably well with the field observations of subsurface contributions to stream flow and the water levels observed in piezometers. Whether the calibrated model can indeed be considered validated is difficult to assess. For example, if this model can accurately predict the check parameters for a subsequent snowmelt period, one could consider that the model is indeed validated. However, difficulties in obtaining reliable field data on the inflow function across the inflow boundary and the sensitivity of the model response to the inflow function, are bound to thwart such a validation procedure. As the authors themselves point out, the value of this case history lies in the recognition that the principal role of this type of mathematical model is to help define more clearly the various mechanisms within the hydrologic cycle so that simpler hydrologic response models can be more firmly based on reality.

An important class of problems related to shallow groundwater systems is that of simulating plant root-soil interactions. Feddes et al. (1975) used the finite-element method to simulate evapotranspiration in an agricultural field in De Groeve, Netherlands. The field in question is covered by peaty soil with an average thickness of about 1.4 m and is underlain by about 10 m of sandy soil. The sandy soil in turn is separated from a deeper aquifer by a 2 m aquitard of clayey soil. The deeper aquifer is intermittently pumped

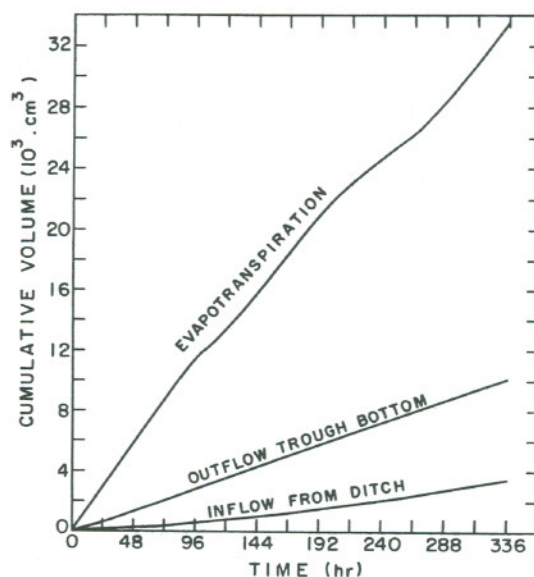


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Fig. 21. Time dependence of boundary conditions, De Groeve finite-element simulation (Feddes et al., 1975).

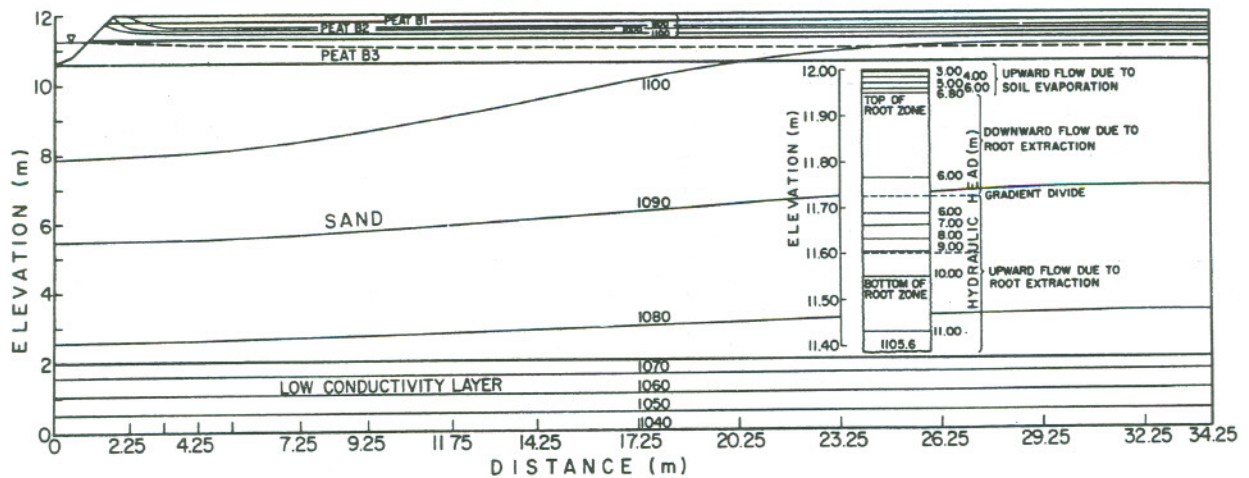
by means of domestic wells outside the area of interest. The field is traversed by several unlined irrigation ditches where water levels can be controlled at will.

Due to symmetry, only one half of the region between two ditches need be considered and a cross section, together with the FEM network, is shown in Fig. 20. The peat and sand layers were assumed to be anisotropic with horizontal permeability ten times the vertical. The root zone is assumed to increase from an initial depth of 40 cm to 50 cm at the end of 168 hours. The water level in the ditch is assumed to be the same as the initial depth of the water table, 74 cm below ground level, and initially the system is assumed to be hydrostatic. The time-dependent hydraulic-head variation in the pumped aquifer as well as the maximum possible rates of soil evaporation and plant transpiration are illustrated in Fig. 21.



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Fig. 22. Computed boundary fluxes, De Groeve finite-element simulation (Feddes et al., 1975).

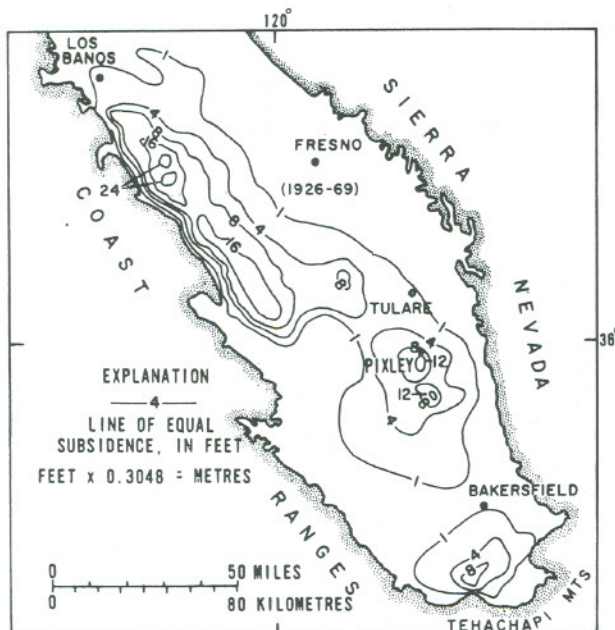


XBL 7611-4764

Fig. 23. Distribution of hydraulic head after 336 hours, De Groeve finite-element simulation (Feddes et al., 1975).

The dynamic numerical simulation extended over a period of 335 hours. Time steps varied from an initial value of 1 hour to 48 hours. Figure 22 shows results for the cumulative fluid fluxes leaving or entering the system due to evapotranspiration, ditch infiltration, and leakage to the underlying pumped aquifer. The distribution of hydraulic heads in the system at the end of 336 hours is shown in Fig. 23. The inset in this figure shows how local upward and downward zones of water movement exist in the uppermost part of the system, and are controlled by evaporation and root extraction.

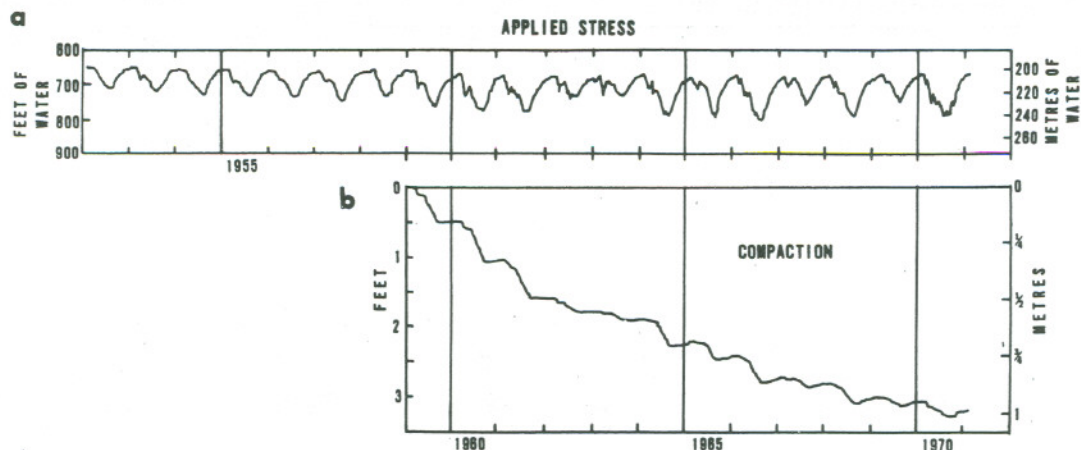
The principal phenomenon of interest in the case histories presented so far has been the movement of water. When hydrogeologists are concerned with the problem of land subsidence due to groundwater extraction, the main phenomenon of interest becomes the movement of the soil skeleton, rather than the movement of water. Helm (1974, 1975) successfully simulated the land subsidence observed at Pixley, California, using the one-dimensional consolidation theory of Terzaghi (1925). The geographic location of the Pixley site and the extent and magnitude of subsidence in the San Joaquin Valley are shown in Fig. 24. The compacting groundwater body at Pixley consists of a sequence of intercalated sands (aquifers) and clays (aquitards) between depths of 355 and 760 ft. Water-level changes in the hydraulically interconnected, highly permeable aquifers are essentially the same and have been systematically observed over two decades by the U.S. Geological Survey. These water-level changes form the boundary conditions controlling drainage (and the consequent compaction) of the aquitards. In addition, since 1959, the compaction of the entire system, down to 760 ft, has been monitored by means of extensometers. The time-dependent changes in water levels (applied stress at the aquitard interface) and the observed compaction are shown in Fig. 25.



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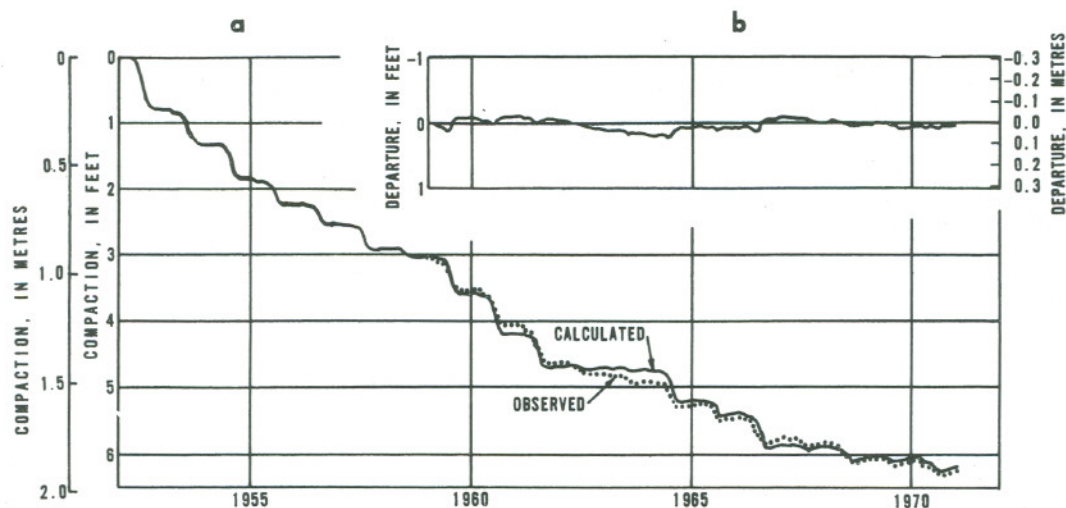
Fig. 24. Extent and magnitude of observed land subsidence, San Joaquin Valley, California (Helm, 1975).

In using a finite-difference model, Helm (1975) assumed that almost all the observed compaction was taking place in the clay and that the clay possessed nonreversible compaction properties. The aquitard parameters, which were constant with time were as follows: permeability = 3×10^{-3} ft/year; recoverable specific storage = 4.6×10^{-6} ft⁻¹ and nonrecoverable specific storage = 2.3×10^{-4} ft⁻¹. As is obvious from Fig. 25, the simulation problem is one of modeling a cyclic boundary condition in conjunction with nonreversible material properties. A comparison of the observed and computed compaction at Pixley is shown in Fig. 26, and it is seen that the agreement between the two is reasonably good considering the complexity of the real system.



XBL 7611-4760

Fig. 25. Field data measured near Pixley, California; a) average applied stress, and b) cumulative compaction (Helm, 1975).



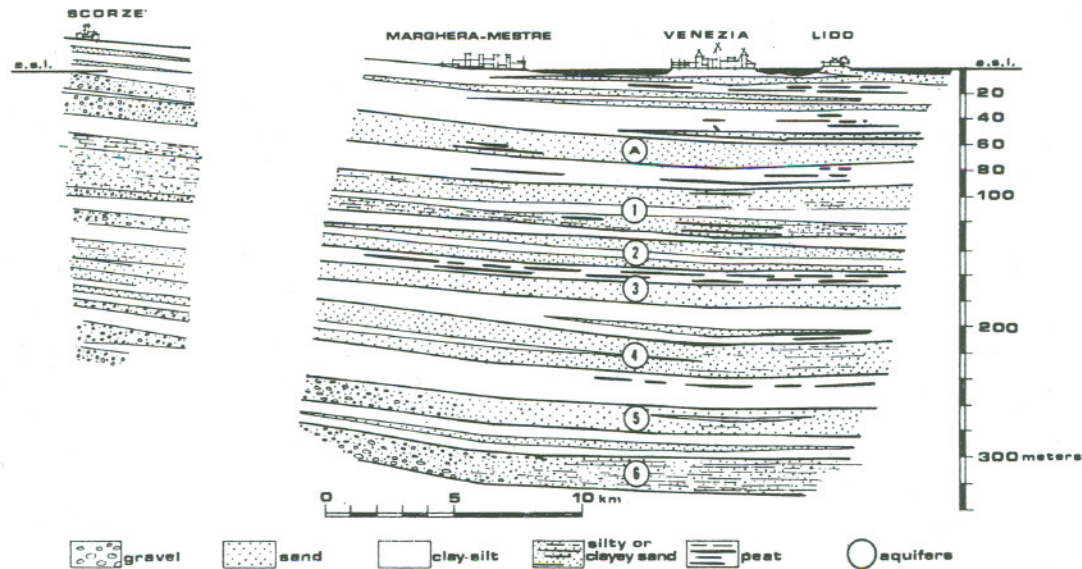
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Fig. 26. Comparison of computed and observed compaction at Pixley, California (Helm, 1975).

The historic city of Venice provides another case history for simulating land subsidence (Gambolati and Freeze, 1973; Gambolati et al., 1974). The city has been sinking at an alarming rate (10 cm during 1952-1969) in recent years mainly due to heavy groundwater withdrawals in the Merghera industrial area about 10 km to the west. The purpose of the mathematical simulation was to correlate subsidence and groundwater withdrawal from past data and then to investigate how the adverse effects of ground settlement could be halted by various programs of modified groundwater management.

The city of Venice is underlain down to about 330 m by a system of sands and silts with interbedded clays (Fig. 27). Although the material

properties of these materials are locally known from laboratory data, their regional properties are not known with any degree of certainty. Due to the sparseness of available field data and the axisymmetric nature of the proposed model, the authors chose to use a dual simulator. This consisted of a finite-element hydrologic model for computing head changes in the aquifers as a function of time and a one-dimensional finite-difference subsidence model for the aquitards, in which the calculated head changes in the aquifers would constitute the boundary conditions. In the hydrologic model, the flow region was divided into a sequence of five aquifers and from intervening aquitards while, in the subsidence model, the vertical column was divided into 20 aquitards. The behavior of the subsidence model is very similar



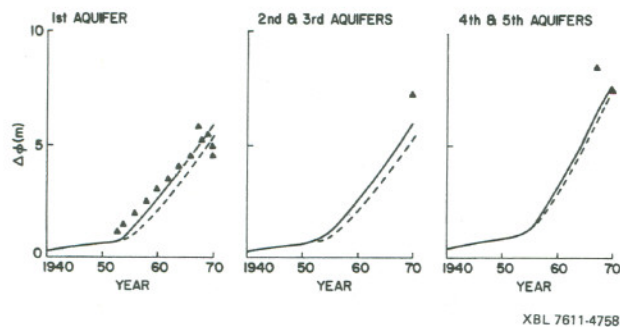
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Fig. 27. Geologic cross section from west to east of the Venice lagoon (Gambolati et al., 1974).

to that of Helm (1974, 1975) in using the Terzaghi theory and in providing for nonrecoverable compressibility coefficients.

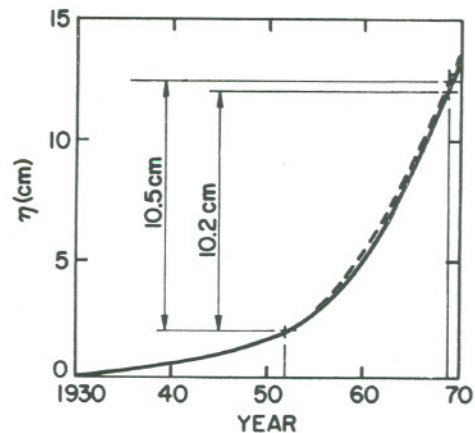
The first task in the simulation was to calibrate the hydrologic model. The calibration procedure was essentially one of trial and error. The following range of parameters was investigated: for the aquifers, permeability 3.2×10^{-3} to 1.6×10^{-2} cm/sec, compressibility 1×10^{-4} cm²/kg; for the aquitards, permeability 1×10^{-6} to 1.6×10^{-5} cm/sec, compressibility 1.5×10^{-3} to 3×10^{-3} cm²/kg. A comparison of the computed

piezometric head declines in the aquifers and the computed subsidence with the historical records up to 1970 is shown in Figs. 28 and 29. Using these calibrated values, the subsidence in Venice was predicted for several future pumping schedules as shown in Fig. 30. The results of the prediction indicated that if the pumping rates are kept constant at present values, a further 3 cm subsidence could be expected to occur in the future. Subsidence could be arrested by reducing the Marghera withdrawal by 25% along with shutting down pumping of the Tronchetto well. Cessation of all pumping would provide a modest rebound of 2 cm.



XBL 7611-4758

Fig. 28. Comparison of observed and computed piezometric head changes at Venice. Dashed lines represent head changes solely due to Marghera pumping. Triangles represent observed values (Gambolati et al., 1974).



XBL 7611-4759

Fig. 29. Computed subsidence at Venice using two different calibration parameters (Gambolati et al., 1974).

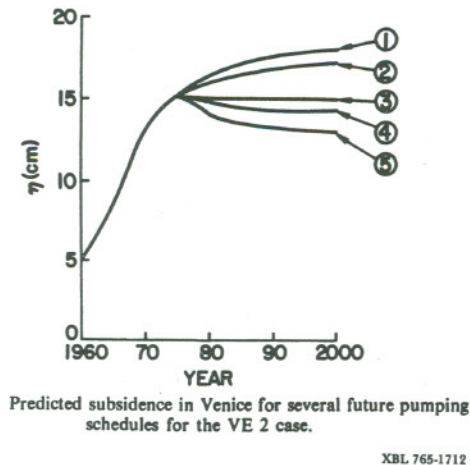


Fig. 30. Predicted subsidence for Venice for several future pumping schedules (Gambolati et al., 1974).

The next case history to be discussed pertains to the use of statistical techniques to establish the spatial variation of material properties in an alluvial basin with meager borehole data. Lippmann (1973) chose this approach to model the Mocho subbasin of the Livermore Valley, California (Fig. 31). The two-dimensional groundwater system simulated was approximately 10,000 ft long and 200 ft thick and was idealized as comprised of 2 materials: a high-permeability material (material 1) containing sand, gravel, boulder, and associated sediments, and a low-permeability material (material 2) containing clay, sandy clay and other clayey sediments. In all, electrical and lithological data were available from the six boreholes distributed over the system. Because the alluvial sediments have been deposited by meandering streams, correlation of adjacent borehole

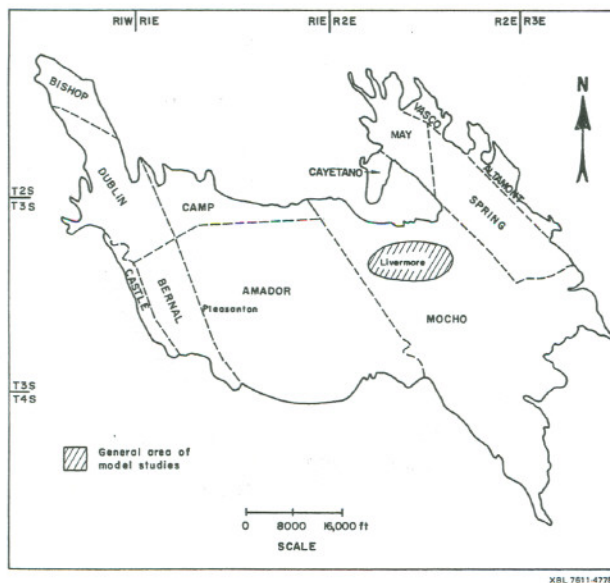


Fig. 31. Groundwater subbasins of the Livermore valley, California (after Lippmann, 1974).

sequences is almost impossible.

In order to achieve a steady-state hydrologic simulation of the basin, Lippmann wanted to compute a statistically equivalent hydraulic conductivity of the system, which, when multiplied by the prevalent hydraulic gradient, would pass the same flux across a unit area as that of the prototype. The calculation of the equivalent hydraulic conductivity was to be done in two steps. The first step was to set up a statistical "Poisson-line" model of the heterogeneous system (Fig. 32) using the probability distribution determined by a Markov chain process of analyzing repetitions at 2-ft intervals as observed in the boreholes. In the second stage, the heterogeneous flow region represented by the Poisson line model was solved for the Laplace equation using simple prescribed boundary conditions.

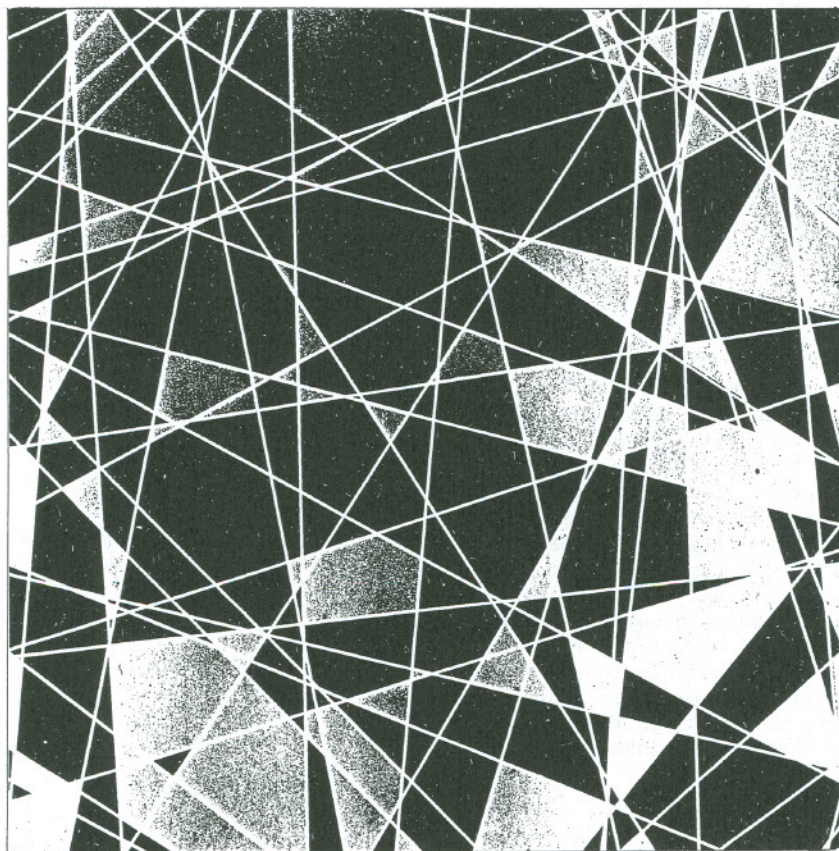
The FEM analysis for potential consisted in matching different-sized networks to the simulated sections. It was found that as the shapes of the elements were changed from squares to rectangles with elongations as much as 1 x 50, the computed flow rates increased. In the absence of appropriate accuracy estimates for the FEM when applied to complex geometries and strong permeability contrasts, it is obvious that the calculated effective hydraulic conductivity is subject to certain model-induced uncertainties. The results obtained from two different FEM meshes are presented in Table II.

The last case history that we shall consider is the application of the inverse method by Emsellem and DeMarsily (1971) to the estimation of transmissivity distribution in an alluvial aquifer of the Rhine River Valley, north of Strasbourg, France. In their parameter identification work, Emsellem and DeMarsily use multiple-objective criteria, instead of minimizing a single-error criterion. Their first objective is to minimize a functional of the residual errors (calibration errors) in a direct formulation of the inverse problem. Their second objective is a criterion for the physical plausibility of the possible solutions. The plausibility criterion used by the authors is that the solution remain uniform (or flat) over the entire flow region. Their approach is to gradually decrease the calibration error by relaxing a certain measure of uniformity until the point is reached when further relaxation of this measure does not cause any substantial reduction in the value of the error functional (Neuman, 1975a).

To test the validity of their method, Emsellem and DeMarsily (1971) first computed the transmissivity distribution in the aquifer by the inverse method, using for input data the known steady-state piezometric head distribution over the area of study. Their results are shown in Fig. 33. Using the transmissivity distribution so calculated, they went on to recalculate the steady-state head distribution over the same basin. A comparison of the computed and observed piezometric heads is shown in Fig. 34. The hatching in the figure represents the difference between computed and observed values and is thus an indication of the calibration error.

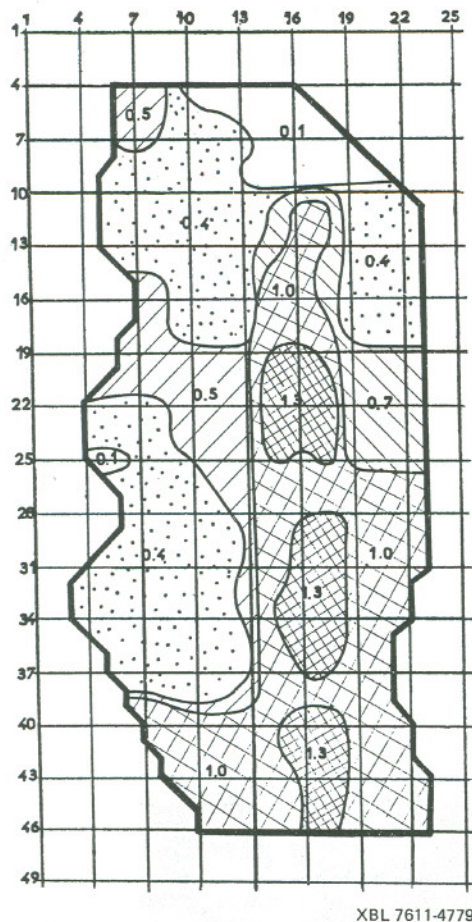
Table II. Results of statistical analysis of data obtained in using 49 x 49 and 16 x 400 finite element meshes.

	Mesh 49 x 49	Mesh 16 x 400
<u>Proportion of Material 1 (p_1)</u>		
Sample mean	0.412	0.412
Sample standard deviation	0.016	0.020
<u>K_E / K_1, expressed in percent</u>		
Sample mean	36.9	20.5
Sample standard deviation	1.74	3.24
Sample correlation coefficient between p_1 and K_E / K_1	0.889	0.775
<u>Flow rate (Q), in gpd/ft</u>		
Sample mean	280	156
Sample standard deviation	13.1	24.6



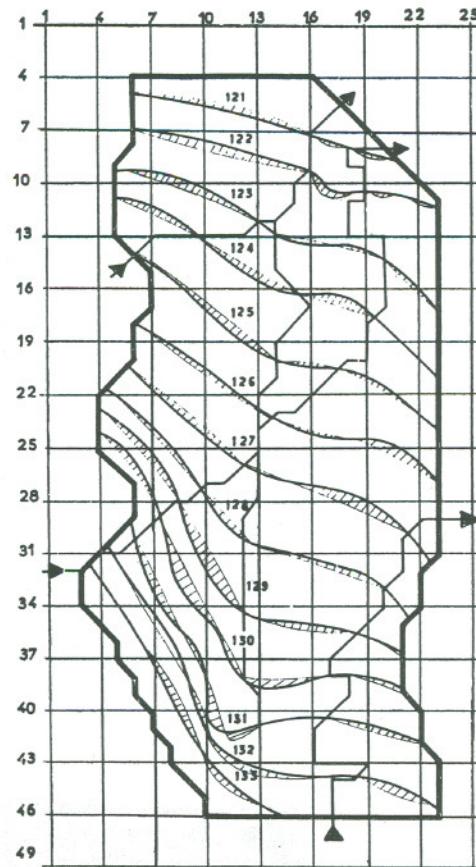
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Fig. 32. Example of a Poisson-line model with material no. 1 shaded (Lippmann, 1973).



XBL 7611-4779

Fig. 33. Distribution of transmissivity over the Rhine aquifer north of Strasbourg, France, computed by the inverse method (Emsellem and de Marsily, 1971).



XBL 7611-4780

Fig. 34. Rhine aquifer, north of Strasbourg, France: comparison of observed heads with those computed using the transmissivity values determined by the inverse method. Shaded area is the difference between the two values (Emsellem and de Marsily, 1971).

CONCLUDING REMARKS

From the survey carried out in this paper, there is little doubt that numerical modeling is now established as a very valuable tool in understanding groundwater systems. The classical finite-difference approach continues to enjoy wide popularity due to its simplicity and its easy extension to nonlinear as well as multidimensional problems. The more recent finite-element method is a powerful technique in handling complex geometry and arbitrary tensorial quantities as well as providing the option of higher-order approximations for the dependent variable in space and time. Due to limitations of computer storage and computational effort, some difficulties exist in applying the FEM to three-dimensional and nonlinear problems.

In considering the future for numerical modeling of regional groundwater systems, the primary question concerns the degree of applicability to actual field situations. It is apparent that the models are most useful when employed in a deterministic manner to synthesize material properties and geometry and to predict the time-dependent response of a given system. Unfortunately, there are some limitations to such applications. First,

the material properties as applied to porous media are macroscopic averages. These averages, combined with the heterogeneity of grain-size distribution in natural sediments, are fundamentally statistical in nature and therefore can not really be represented by deterministic values. Secondly, the sparsity of samples introduces a statistical element in the parameters used in the regional model. It is quite apparent that laboratory measurements and other small-scale experiments used for parameter estimation are inadequate for arriving at the distribution of material properties over the global system.

There is thus a significant trend in attempting to apply inverse methods of parameter estimation and this trend will definitely be pursued in the future. The trial and error methods of parameter estimation used in many of the case histories described here constitute the intuitive and simple approach to the inverse problems. The more sophisticated techniques of linear and quadratic programming seek to achieve a more rational and efficient method of model parameter estimation. Much continued activity in the use and improvement of these techniques can be expected in the future.

It should be remembered that the process of obtaining a solution to a parameter estimation problem actually consists of choosing a most plausible solution from a class of non-unique solutions. In order that a most reasonable choice be made, it is imperative that a good knowledge of the geologic makeup of the field system is forthcoming. Thus, the mathematical model in itself does not constitute an effective tool of analysis unless it complements field observations.

Apart from the ability of predicting the response of real systems to various plausible input functions, and of identifying system parameters, numerical models have a very special and very powerful advantage. This results from the fact

that by simulating various hypothetical situations numerically, one should be able to more clearly define the actual mechanisms that control a given complex field situation.

Until now, mathematical models have been employed principally for predicting groundwater flow patterns and, to a lesser extent, for parameter estimation. The power of the models, however, has not been utilized to study problems related to the important aspects of groundwater prospecting, design of data collection networks and instrumentation. There is little doubt that numerical models have a lot to offer in regard to understanding these areas of hydrogeology.

NOMENCLATURE

$[A]$	conductance or "stiffness" matrix		$\vec{q}_r$	vector flux density of water relative to the solid grains of the porous medium	$[L^3/T]$
a	a matrix-fracture coefficient	$[1]$	$\{Q\}$	vector of source terms	
C	specific moisture capacity	$[1/L]$	r_s	radius of skin	$[L]$
C_c	compression index	$[1]$	r_w	radius of well	$[L]$
C_s	swelling index	$[1]$	S	saturation	$[1]$
D	soil moisture diffusivity	$[L^2/T]$	s_s	specific storage	$[1/L]$
$D_{n,m}$	distance between nodal points n and m	$[L]$	s_y	specific yield or effective porosity	$[1]$
$[D]$	nondiagonal capacity matrix		t	time	$[T]$
$[D^*]$	diagonal capacity matrix		v	prescribed specific flux	$[L/T]$
e	void ratio	$[1]$	V	bulk volume of a volume element	$[L^3]$
E	potential evaporation	$[L^3/T]$	V_s	volume of solids	$[L^3]$
E^*	potential evapotranspiration	$[L^3/T]$	V_v	volume of voids	$[L^3]$
g	gravitational constant	$[L/T^2]$	w_f	fracture width	$[L]$
G	volumetric rate of fluid generation per unit volume	$[L^3/L^3T]$	z	elevation	$[L]$
h	hydraulic head	$[L]$	α	volumetric compressibility of soil skeleton (synonymous with m_v of soil mechanics literature)	$[LT^3/M]$
h'	approximate value of h	$[L]$	β	volumetric compressibility of water	$[LT^2/M]$
k	absolute permeability or specific permeability tensor	$[L^2]$	γ_w	specific weight of water	$[M/L^4T^2]$
K	hydraulic conductivity or permeability	$[L/T]$	Γ	boundary surface of a volume element v	$[L^2]$
k_f	hydraulic conductivity of fracture	$[L/T]$	θ	volumetric moisture content	$[1]$
k_s	hydraulic conductivity of skin	$[L/T]$	λ	weighting factor for backward differencing	$[1]$
L_f	fracture length	$[L]$	ξ	elevation of the freesurface above the base	$[L]$
m_c	specific fluid mass capacity	$[M/LL^3]$	ρ_w	mass density of water	$[M/L^3]$
M_c	fluid mass capacity of an element with volume V	$[M/L]$	σ	total stress on soil skeleton	$[M/LT^2]$
M_{nm}	magnitude of mass transfer into subdomain n from subdomain m	$[M]$	σ'	effective stress on soil skeleton	$[M/LT^2]$
M_w	mass of water contained in a volume element of bulk volume V	$[M]$	X, X'	parameter relating pore fluid pressure and effective stress	$[1]$
n	porosity	$[1]$	ψ	pressure head	$[L]$
$\vec{n}$	a unit outer normal of the surface segment $d\Gamma$	$[1]$	ψ_A	air entry value	$[L]$
$\vec{n}_z$	unit vector parallel to z axis	$[1]$	ψ_w	wilting coefficient of root system	$[L]$
p	pore fluid pressure	$[M/LT^2]$			
$\vec{q}$	specific flux vector of Darcy velocity	$[L^3/T]$			

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*This work supported by the U.S. Energy Research and Development Administration.

This report was done with support from the United States Energy Research and Development Administration. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the United States Energy Research and Development Administration.