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MATHEMATICAL DEVELOPMENT AND VERIFICATION OF A FINITE ELEMENT AQUIFER FLOW MODEL AQUIFEM-1

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PREFACE

This report is one of a series of publications which describe various studies undertaken under the sponsorship of the Technology Adaptation Program at the Massachusetts Institute of Technology.

In 1971, the United States Department of State, through the Agency for International Development, awarded the Massachusetts Institute of Technology a grant. The purpose of this grant was to provide support at M.I.T. for the development, in conjunction with institutions in selected developing countries, of capabilities useful in the adaptation of technologies and problem-solving techniques to the needs of those countries. At M.I.T., the Technology Adaptation Program provides the means by which the long-term objective for which the A.I.D. grant was made, can be achieved.

Fred Moavenzadeh
Program Director

ABSTRACT

MATHEMATICAL DEVELOPMENT AND VERIFICATION
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The mathematical development of a two-dimensional finite element model for groundwater flow is described. Based on the hydraulic equations of essentially horizontal flow, the model is called AQUIFEM-1, Aquifer Finite Element Model-1 Layer. It employs the Galerkin finite element technique, with linear interpolation functions and triangular elements. Leakage from an adjacent aquifer, pumping and recharge wells, lateral inflows and outflows, induced infiltration, and numerous other boundary conditions are accounted for. Both steady state and transient solutions can be computed.

The model is verified by comparison to a variety of steady state and transient analytical solutions. These include 1D steady flow in confined leaky and non-leaky aquifers, and in a phreatic aquifer; 1D transient flow in confined and phreatic aquifers; and 2D radial flow to a well in a leaky and non-leaky confined aquifer, and an aquifer undergoing a change of status.

ACKNOWLEDGMENTS

The final version of AQUIFEM-1, mathematically developed and verified in this report, was sponsored by the M.I.T. Technology Adaptation Program under OSP Project 85054, which is funded through a grant from the Agency for International Development, U.S. Department of State. The views and opinions expressed in this report, however, are those of the authors and do not necessarily reflect those of the sponsor.

Acknowledgment must also be given to the staff and Executive Committee of the M.I.T./Cairo University Technology Planning Program, for their support of the Nile Delta Groundwater Study, the project for which this revised model was prepared. In particular, Professors Mohamed Hashish and Emad Rasmy suggested useful improvements to the code. An earlier version of AQUIFEM was developed as part of a joint M.I.T./Tippetts-Abbett-McCarthy-Stratton project for the integrated development of the Vardar/Axios River Basin (Yugoslavia and Greece) sponsored by the UNDP under OSP project 83355.

A special word of thanks goes to Ms. Carole Solomon for her patience and excellent typing of this report.

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Chapter 1

INTRODUCTION

In planning water resources projects involving the use of groundwater, it is important to understand the behavior of the groundwater system under different alternative policies or operational schemes. Conceptual models in the form of mathematical expressions have been developed to represent this behavior. Most of these expressions are partial differential equations with various types of boundary conditions, some of which represent interaction with surface water. The complex geometry, porous medium properties and boundary conditions inherent in natural aquifer systems make it difficult, if not impossible, to obtain an exact analytical solution for these equations. In the past electrical analog techniques were developed to circumvent this difficulty. With the advent of high speed digital computers, a variety of efficient numerical techniques appeared, followed by a series of numerical models to solve groundwater flow problems.

1.1 Numerical Models

The first technique applied was the *finite difference method* of numerical solution, in which the derivatives in the governing equation of groundwater flow are replaced by difference approximations. Among the most popular models of this type at present are the Illinois State Water Survey Model (Prickett and Lonnquist, 1971) and the U.S. Geological Survey 2-Dimensional Flow Model (Trescott et al., 1976).

In the last ten years the *finite element method* has been applied

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to groundwater problems. In this method the governing partial differential equation is integrated over the aquifer region and the divergence theorem is used to simplify the resulting equation. This *weak form* of the equation is equivalent to the original equation and has the same solutions. An approximate solution of the weak form is then obtained by assuming that the piezometric head can be expressed in terms of piecewise continuous polynomials. The method has several advantages over the finite difference technique, for example:

i) a better description of irregular boundaries, without the need for special formulas;

ii) the ease of employing an irregular grid to provide different levels of spatial discretization in different regions of the aquifer;

iii) aquifer non-homogeneity and anisotropy are easily handled;

iv) fewer node points are sometimes required to represent the aquifer to the same level of accuracy, resulting in savings of computational time and computer storage.

Several finite element models are already available for groundwater flow problems. Among them are those developed by Gupta et al. (1975, 1976), Pinder (1972, 1976), and Narasimhan et al. (1978).

A summary of numerical models used by the U.S. Geological Survey is found in Appel and Bredehoeft (1976), and a more general summary of groundwater models can be found in the report prepared for the Environmental Protection Agency (1978). For the reader less familiar with numerical methods, Forsythe and Wasow (1960) and Remson et al.

(1971) provide background in finite difference simulation, the latter applied to groundwater. Zienkiewicz (1977), Desai and Abel (1972), Huebner (1975), Connor and Brebbia (1976) and Pinder and Gray (1977) describe the finite element method. The last two of these references contain special sections dedicated to groundwater flow modeling.

1.2 AQUIFEM-1

The purpose of the present report is to present the mathematical development and verification of a simple and inexpensive two dimensional finite element model of groundwater flow: AQUIFEM-1, an acronym for AQUIfer Finite Element Model-1 layer. A description and user's manual for the AQUIFEM-1 computer code is provided in a companion report by Townley and Wilson (1980).

The typical management problem for which a groundwater model is required is that involving a single aquifer which can be represented by a two dimensional aquifer hydraulic equation assuming essentially horizontal flow. This type of aquifer may be phreatic or confined, or a combination of these conditions, and may be subject to leakage. Groundwater managers may need to assess aquifer/river interaction, artificial recharge, and the development and operation of pumping wells; to study locations for observation wells and pumping tests; or to investigate policies for safe yield and/or conjunctive use. AQUIFEM-1 has been designed to study these kinds of problems.

The following objectives were considered in the development of AQUIFEM-1:

1) Simplicity - the model should require no special background in numerical methods for the user familiar with groundwater hydraulics;
   - the model should be capable of running on a mid-size computer, say 40K words or more, depending on the number of nodes;
   - special packages for scientific subroutines should not be required;
   - (These objectives stem from the wish to make the model easily and widely applied in countries less developed than the United States.)
2) Accuracy - the solutions obtained by AQUIFEM-1 should be as accurate as possible, consistent with the reliability of the data and the adequacy of the conceptual model (governing equations) of the aquifer.
3) Applicability to field problems - because these are the problems decision makers face and for which they require the expertise of the groundwater hydrologist and/or geologist.
4) Versatility - the model should be capable of handling a variety of problem situations usually encountered in the field.

In accordance with these objectives, AQUIFEM-1 is a finite element model using the Galerkin technique with triangular elements and linear interpolation functions, for anisotropic and non-homogeneous, phreatic or confined, leaky or non-leaky aquifers. Aquifer properties and boundary condition values are assumed to be constant* within individual elements and *lumping* techniques are used to simplify matrices. The model can analyze both steady and unsteady behavior using unconditionally convergent algorithms.

Model formulation has three basic steps which are described in the following three chapters. A considerable amount of detail is given in order to reduce the need for other references. In Chapter 2 the governing equation for two dimensional horizontal flow in an aquifer is presented along with the assumptions behind its derivation and appropriate boundary conditions. Chapter 3 presents the finite element method, based on the Galerkin technique with linear triangular elements, which is used to integrate the governing differential equation in space. Lastly, Chapter 4 presents the method of solution of the matrix equation for both steady and unsteady problems. In Chapter 5 the model is theoretically verified by comparing numerical and analytical solutions of simple groundwater flow problems.

An earlier out-of-date version of AQUIFEM-1 is described by Sa da Costa (1978). A User's Manual and Description of the current version (November 1979) of AQUIFEM-1 is given in Townley and Wilson (1980).

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*There are certain exceptions to this rule, when transmissivity and storage coefficient are allowed to vary over the elements (see Section 3.9).

Chapter 2

GOVERNING EQUATION

The governing differential equation for two-dimensional groundwater flow in a non-homogeneous, anisotropic aquifer with leakage is (Bear, 1972, 1979):

$$S \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left(T_{xx} \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y} \left(T_{yy} \frac{\partial h}{\partial y}\right) + Q + \frac{K'}{B'} (h_a - h) \qquad (2.1)$$

where certain terms are defined in Figure 2.1 and:

$S = S(x,y,t)$ = aquifer storage coefficient [-];

$h = h(x,y,t)$ = depth averaged piezometric head, usually denoted ϕ for confined aquifers [L];

$T_{xx} = T_{xx}(x,y,t)$ = aquifer transmissivity in the x-direction, $[L^2/T]$;

= $K_{xx}(x,y)B(x,y)$ for confined aquifers, where K_{xx} is the hydraulic conductivity [L/T] and B is the aquifer thickness [L];

or = $K_{xx}(x,y)[h(x,y,t)-z(x,y)]$ for phreatic aquifers, where z is the aquifer bottom elevation and (h-z) is the saturated thickness;

$T_{yy} = T_{yy}(x,y,t)$ = aquifer transmissivity in the y-direction given by $K_{yy}B$ or $K_{yy}(h-z)$ as above, $[L^2/T]$;

$Q = Q(x,y,t)$ = net vertical flux into the aquifer from point or distributed sources (or sinks) (e.g., wells, irrigation or evapotranspiration), [L/T];

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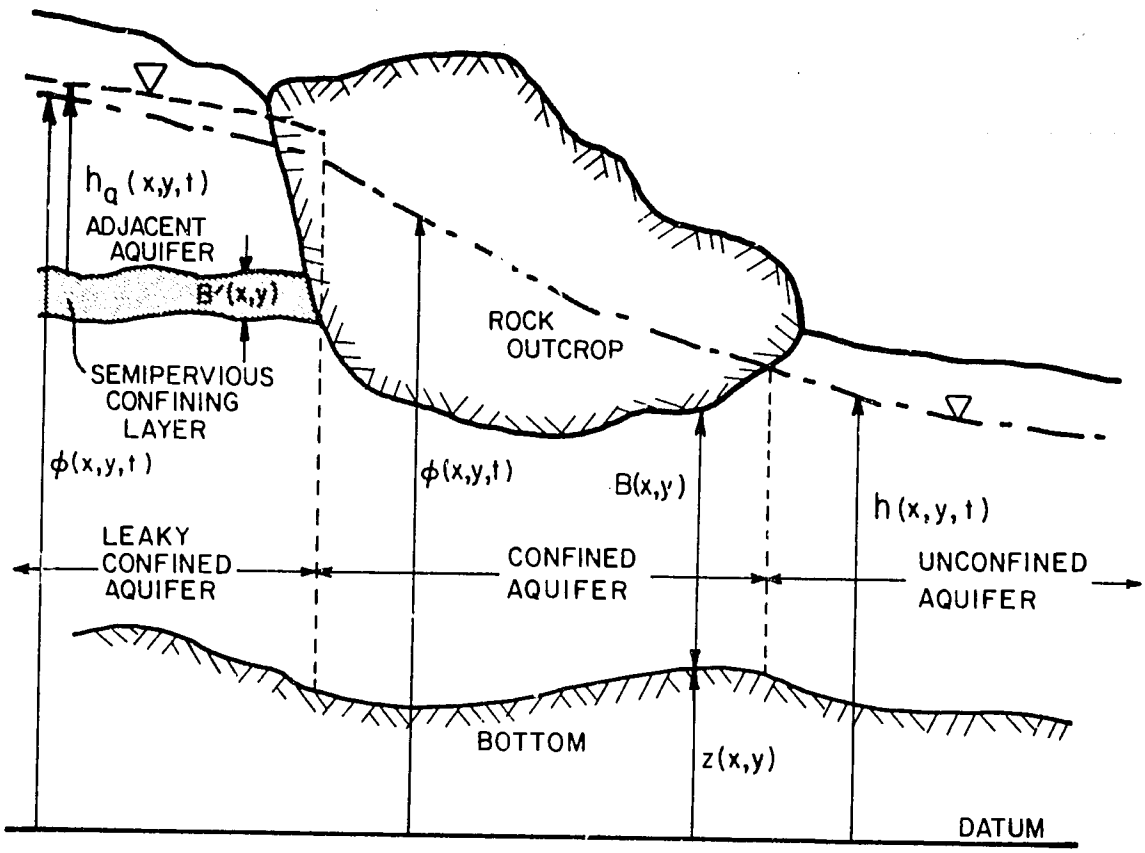


— · — · — Depth-averaged piezometric head (Water table in unconfined aquifer)

- - - - - - - Depth-averaged piezometric head in adjacent aquifer (Water table if adjacent aquifer is unconfined)

Figure 2.1 Definition Sketch - Cross-section of a Hypothetical Aquifer.

$K' = K'(x,y)$ = vertical permeability of a semi-pervious layer above or below the aquifer, [L/T], (only one such layer is allowed in AQUIFEM-1);

$B' = B'(x,y)$ = thickness of the semi-pervious layer above or below the aquifer, [L];

$h_a = h_a(x,y,t)$ = piezometric head in an adjacent aquifer separated from the main aquifer by the semi-pervious layer [L];

x,y = Cartesian coordinates (principal axes of the hydraulic conductivity/transmissivity tensor) [L];

and t = time [T].

The following assumptions are made in the derivation of Eq. 2.1:

1) The water is considered to be a homogeneous fluid with constant density;
2) Darcy's Law is applicable;
3) The Dupuit approximation is assumed valid, therefore the flow is essentially horizontal. Vertical flow is only considered in the semi-pervious layer in the presence of leakage;
4) The off-diagonal terms of the transmissivity tensor, $T_{xy}=T_{yx}$, are zero (x and y are principal axes);
5) The aquifer storage is attributable only to specific yield, S_y, if phreatic, or to elastic storativity, S_oB, if confined, where S_o is specific storativity; and
6) there is no time-dependent release of water from storage inside the semi-pervious layer.

The aquifer domain may be anisotropic and non-homogeneous with respect to hydraulic conductivity (or transmissivity) and non-homogeneous with respect to the storage coefficient.

Three types of boundary conditions for Eq. 2.1 are generally encountered in groundwater flow problems. The first type requires the prescription of the piezometric head, h, and is used to model lakes, rivers or streams which fully penetrate the aquifer under study. The second type of boundary condition prescribes the water flux across the aquifer boundary which is proportional to the first spatial derivative of head normal to the boundary. Prescribed flows are used when there is lateral flow between the aquifer and an adjacent region, and in particular when there is no such flow. The distinction between these lateral boundary fluxes which are boundary conditions for Eq. 2.1, and vertical inflows represented in Eq. 2.1 by the terms $Q(x,y,t)$ and $(K'/B')(h_a-h)$ is important and is discussed in detail by Bear (1979). The third type of boundary condition defines a relationship between the head outside the aquifer and the flux across the boundary. It is used to model lakes and rivers which are partially penetrating or which are lined with a semi-pervious (silty) layer. For convenience the three types of boundary conditions described above are designated in this report as 1st, 2nd and 3rd-type boundary conditions, respectively. Figure 2.2 illustrates the definition of boundary segments Γ_1, Γ_2 and Γ_3. The term *domain* in the figure refers to the area of the aquifer being modeled; it is coincident with the solution domain of Eq. 2.1 and is denoted Ω in this report.

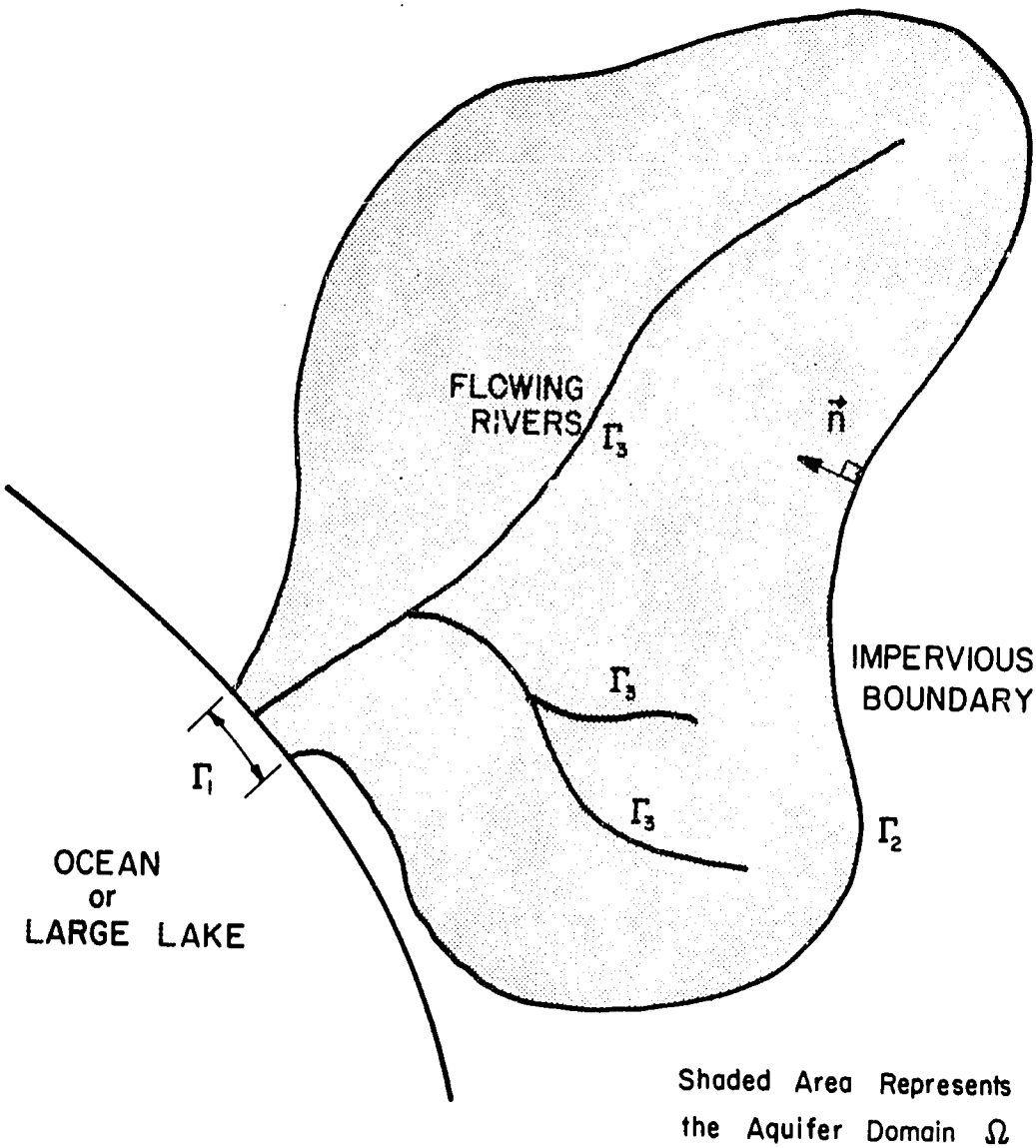


Figure 2.2 Example Aquifer Domain.

The boundary conditions for Eq. 2.1 can all be described mathematically. The prescribed head or 1st-type boundary condition is also variously called a Dirichlet, essential or geometric boundary condition and is given by:

$$h = h_1(x,y,t) \tag{2.2}$$

on the appropriate boundary segment, Γ_1. The prescribed flux or 2nd-type boundary condition is described by the terms Neumann, natural or force boundary condition and is given by:

$$-(T_{xx} \frac{\partial h}{\partial x} n_x + T_{yy} \frac{\partial h}{\partial y} n_y) = Q_s(x,y,t) \tag{2.3}$$

along the boundary segment Γ_2, where n_x and n_y are the x and y components of the unit inward-pointing normal vector $\vec{n}$ on Γ_2 and Q_s is an inflow per unit length $[L^2/T]$. The mixed or 3rd-type boundary condition is given by:

$$-(T_{xx} \frac{\partial h}{\partial x} n_x + T_{yy} \frac{\partial h}{\partial y} n_y) = (\frac{K''W''}{B''})(h_3-h) \tag{2.4}$$

along the boundary segment Γ_3, where n_x and n_y are again components of the inward pointing normal vector $\vec{n}$ on Γ_3, and the right hand side represents the inflow per unit length due to a known head h_3 outside the aquifer. Conceptually, K" is the equivalent hydraulic conductivity of a leaky zone on Γ_3 which has an effective depth (in the direction of leaky inflow) B" and width (perpendicular to the inflow) W". In practice, however, the parameter (K"W"/B") is usually given as a single value.

For transient flow problems Eq. 2.1 also requires an initial condition in which the piezometric head is specified over the entire aquifer domain at time t_o:

$$h = h_o(x,y,t_o) \quad \text{at} \quad t = t_o \tag{2.5}$$

If the initial condition is not itself a steady state solution of Eq. 2.1, there are some additional complications since initial unsteady effects must also be accounted for.

AQUIFEM-1 is designed to solve the governing equation (Eq. 2.1) subject to boundary and initial conditions (Eqs. 2.2 to 2.5) where aquifer properties and boundary conditions have spatial and temporal variations as implied in the definitions above. Most of the model's capabilities are relatively straightforward applications of the finite element method to these equations, subject to time-varying parameters. Other common situations not yet mentioned, however, can also be approximately analyzed:

1) The case where an aquifer changes status at some location from confined to unconfined (or vice versa) and undergoes a very large local change in the aquifer storage coefficient.
2) The case where the water table in an unconfined aquifer rises to ground level and can rise no further. The aquifer at such a location is effectively part of the 1st-type boundary, at least until there is a tendency for the water table to fall again.
3) The case in which the water table drops below the bottom of a partially penetrating stream and the rate of induced infiltration becomes constant or base flow to stream becomes zero. The stream

boundary effectively changes from a 3rd-type boundary to a 2nd-type boundary in this case.

4) The case of a flowing well in which the piezometric head of an artesian aquifer drops below land surface elevation, and the well discharge ceases. The 1st- or 3rd-type boundary condition has effectively been removed until the head rises again.

5) The case of evapotranspiration dependent on the water-table elevation.

6) The case of an excavation with sump or pit dewatering in which the land surface elevation is sequentially lowered into a phreatic aquifer. This results in a progressive 1st-type or 3rd-type boundary which is activated only when the piezometric head exceeds the elevation of the pit bottom.

These and similar situations are not discussed in depth in this report since the complications are computational rather than conceptual. For the details of these features of AQUIFEM-1 see Townley and Wilson [1980].

Chapter 3

FINITE ELEMENT FORMULATION

3.1 General Considerations

Problems in continuous domains, as is the case of an aquifer, have an infinite number of unknowns, each one corresponding to the value of the field variable at each one of the infinite points within the aquifer domain. For groundwater problems the field variable is the piezometric head. In order to make the problem soluble the domain is discretized to give a finite number of unknowns. One way of performing this discretization is to subdivide the domain into a number of cells or elements defined by a certain number of points, called nodes. Within each element the field variable is expressed in terms of its values at the node points and assumed approximation functions between nodes. These functions are commonly known as shape or interpolation functions because they interpoate the value of the field variable between nodes, inside each element. Once the interpolation functions are known for each element, the behavior of the piezometric head over the entire domain is obtained by *assembling* all the elements. The degree of accuracy of the solution depends on the size and shape of the elements, and on the type of interpolation functions. The method described is called the finite element method.

In practical terms, the finite element method can be summarized in six steps:

1) Discretize the domain into elements: as illustrated in

Fig. 3.1 using for example, triangular elements. Other shapes of elements with linear or curvilinear sides are often used.

2) Select a particular finite element approach: that is, choose a method of defining weighting functions w which control the degree of approximation of the method. Different choices of w result in the collocation method, the method of least squares and the Galerkin finite element method.

3) Derive finite element matrix equations: by first deriving the weak form of the problem from the differential equation of interest and then by approximating the solution as a linear combination of shape or interpolation functions.

4) Select interpolation functions: polynomials are usually employed because they are easy to differentiate and integrate. The order of the polynomial depends on the number of nodes defining an element and on its shape. Interpolation functions cannot be taken arbitrarily, because they must satisfy certain continuity conditions within and between elements.

5) Assemble element and global matrices: terms which make up the *global* matrix equations can be expressed in terms of element matrices which depend on the geometry of the elements, the choice of interpolation functions, the element material properties and lastly on boundary conditions. These element matrices are combined to form the global matrix equation which describes the relationship between the unknown field values at all the nodes.

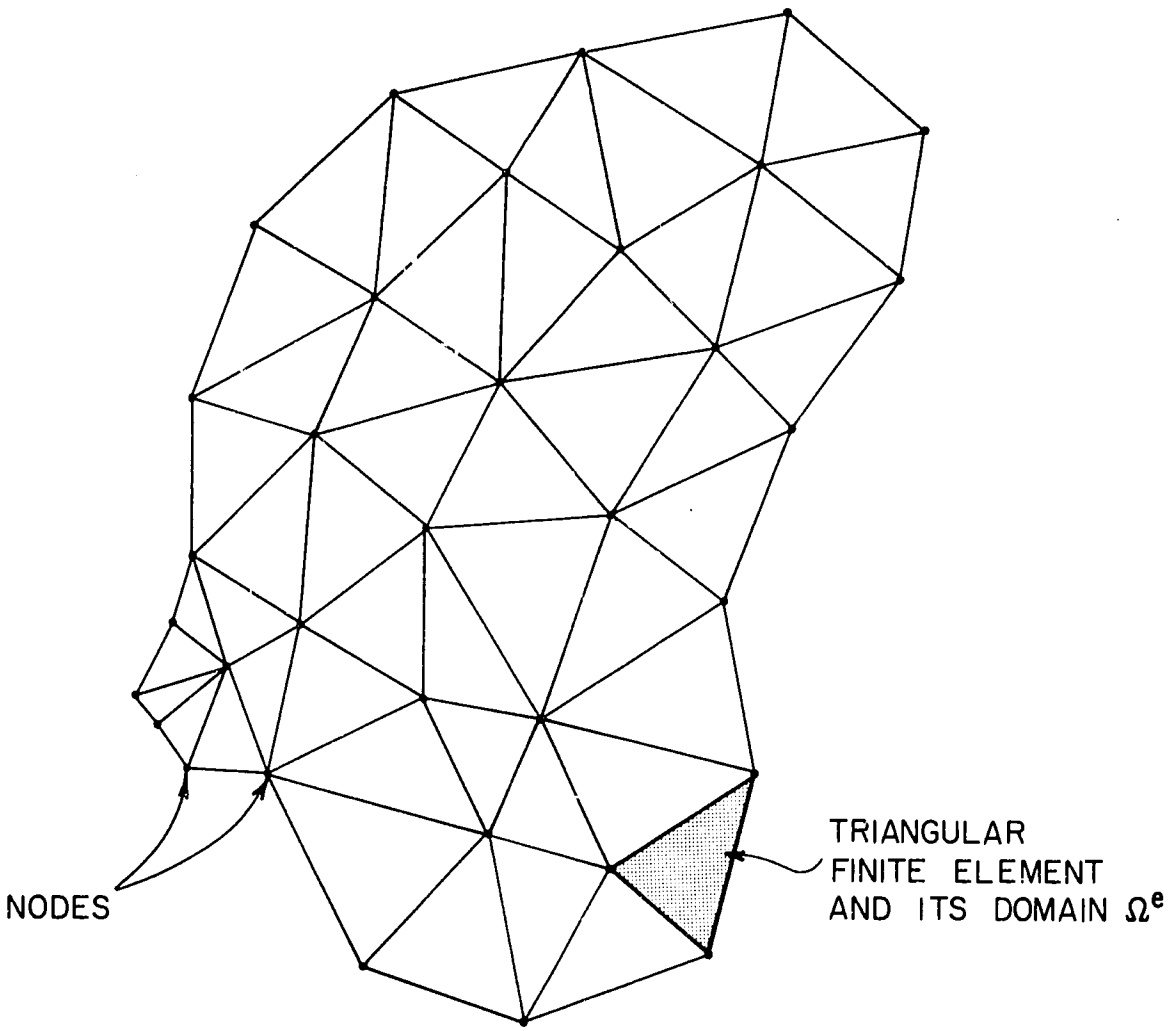


Figure 3.1 Discretization of the Aquifer Domain.

6) Solve the system of equations: different types of algorithms are available to solve the system of equations. Their selection is based on the type of problem and the effectiveness of each algorithm to handle that particular situation.

The formulation of AQUIFEM-1 was guided by the goal of obtaining a simple, effective, versatile and inexpensive finite element code which does not require a large computer system. A secondary goal was that the model be easy to understand and implement, even by users unfamiliar with numerical methods. These goals led to the following choices which are required in the general procedures outlined above. AQUIFEM-1 uses *triangular elements*, like those illustrated in Fig. 3.1, because they are the simplest elements for two dimensional space domains, and flexible enough to accurately represent most geometric boundaries encountered in groundwater flow problems. *Linear interpolation functions* were also selected because of their simplicity and their ability to accurately represent the spatial distribution of piezometric head. Finally, as discussed below, the Galerkin finite element approach was chosen as the particular kind of finite element approximation.

Within the class of finite element methods, three different techniques are commonly used. The differences depend on a particular choice of weighting functions which will become clear in the following sections.

1) Collocation method: in this technique the governing equation is exactly satisfied only at the nodes. It is usually used for problems with few nodes because it leads to non-symmetric, positive

semi-definite systems of equations, which are expensive to solve.

2) Least squares method: in this technique the deviation between the exact and approximate solution, also called the residual error, is minimized over the entire domain in a least squares sense. Although the final system of equations is symmetric, it remains positive semi-definite.

3) Galerkin method: in this technique the interpolation functions and the weighting functions are the same. The final system of equations is then symmetric and positive definite, and is conveniently solved via computer.

As in most finite element codes, the Galerkin method is used in AQUIFEM-1 because of its symmetry and positive definiteness properties. These properties allow the use of a very efficient equation solving method known as a symmetric *profile* or *skyline* solver, which takes advantage of the structure of the generated matrices.

In summary AQUIFEM-1 can be described as a two dimensional finite element model for horizontal groundwater flow which employs triangular elements, linear interpolation functions and a finite element formulation using the Galerkin technique. The remainder of Chapter 3 describes the application of this finite element method in the spatial domain $\Omega(x,y)$ to obtain a set of approximate simultaneous 1st-order ordinary differential equations in time. Chapter 4 describes the solution of these equations in time using a finite difference technique.

3.2 The *Weak* Form of the Problem

The governing equation, Eq. 2.1, can be written in a general form as

$$L(h) - f = 0 \tag{3.1}$$

where L( ) is a linear differential operator, h is the piezometric head and the function f is related to known distributed sources, sinks and leakage. Since this equation is valid at all points in the domain of interest, Ω, it follows that multiplying the equation by some weighting function w gives

$$w[L(h)-f] = 0 \tag{3.2}$$

at all points in Ω. Furthermore,

$$\int_{\Omega} w[L(h)-f]d\Omega = 0 \tag{3.3}$$

since the integrand is identically zero at all points. Eq. 3.3 applies exactly when h is the exact solution of Eq. 2.1.

Writing Eq. 2.1 in this way gives

$$\int_{\Omega} w[S \frac{\partial h}{\partial t} - \frac{\partial}{\partial x} (T_{xx} \frac{\partial h}{\partial x}) - \frac{\partial}{\partial y} (T_{yy} \frac{\partial h}{\partial y}) - Q - \frac{K'}{B'} (h_a - h)]d\Omega = 0 \tag{3.4}$$

This result can be simplified using the divergence theorem (Hildebrand, 1976):

$$\int_{\Omega} \vec{\nabla} \cdot \vec{v} \, d\Omega = -\int_{\Gamma} \vec{v} \cdot \vec{n} \, d\Gamma \tag{3.5}$$

where $\vec{\nabla} = \frac{\partial}{\partial x} \vec{i} + \frac{\partial}{\partial y} \vec{j}$, the gradient operator,

$\vec{v} = v_x\vec{i} + v_y\vec{j}$, an arbitrary vector-valued function on Ω,

$\vec{n} = n_x\vec{i} + n_y\vec{j}$ is the <u>inward</u> pointing unit normal vector on Γ,

and

the arrow over quantities above denotes a vector quantity in (x,y) space.

Substituting

$$\vec{v} = w(T_{xx}\frac{\partial h}{\partial x}\vec{i} + T_{yy}\frac{\partial h}{\partial y}\vec{j}),$$

a particular choice of the vector function $\vec{v}(x,y)$, leads to

$$\int_\Omega w[\frac{\partial}{\partial x}(T_{xx}\frac{\partial h}{\partial x}) + \frac{\partial}{\partial y}(T_{yy}\frac{\partial h}{\partial y})]d\Omega$$

$$= -\int_\Omega(\frac{\partial w}{\partial x}T_{xx}\frac{\partial h}{\partial x} + \frac{\partial w}{\partial y}T_{yy}\frac{\partial h}{\partial y})d\Omega - \int_\Gamma w(T_{xx}\frac{\partial h}{\partial x}n_x + T_{yy}\frac{\partial h}{\partial y}n_y)d\Gamma \tag{3.6}$$

Hence Eq. 3.4 becomes

$$\int_\Omega(wS\frac{\partial h}{\partial t} + \frac{\partial w}{\partial x}T_{xx}\frac{\partial h}{\partial x} + \frac{\partial w}{\partial y}T_{yy}\frac{\partial h}{\partial y} + w\frac{K'}{b'}h)d\Omega$$

$$=\int_\Gamma[-w(T_{xx}\frac{\partial h}{\partial x}n_x + T_{yy}\frac{\partial h}{\partial y}n_y)]d\Gamma + \int_\Omega w(Q + \frac{K'}{B'}h_a)d\Omega \tag{3.7}$$

where the highest derivatives now have order one. The integral over the boundary Γ can be rearranged by splitting the integral into three integrals over Γ_1, Γ_2 and Γ_3. Since $\frac{\partial h}{\partial x}$, $\frac{\partial h}{\partial y}$ are not known *a priori* on the specified head boundary Γ_1, the allowable functions w are restricted by <u>requiring</u> $w = 0$ on Γ_1. The boundary conditions on Γ_2 (Eq. 2.3) simplify the integrand to wQ_s on Γ_2, and similarly on Γ_3 (see Eq. 2.4), the integrand reduces to $w(\frac{K''W''}{B''})(h_3-h)$. Thus

$$\int_\Omega \left(wS \frac{\partial h}{\partial t} + \frac{\partial w}{\partial x} T_{xx} \frac{\partial h}{\partial x} + \frac{\partial w}{\partial y} T_{yy} \frac{\partial h}{\partial y} + w \frac{K'}{B'} h\right) d\Omega + \int_{\Gamma_3} w \frac{K''W''}{B''} h d\Gamma_3$$

$$= \int_{\Gamma_2} wQ_s d\Gamma_2 + \int_{\Gamma_3} w \frac{K''W''}{B''} h_3 d\Gamma_3 + \int_\Omega w\left(Q + \frac{K'}{B'} h_a\right) d\Omega \qquad (3.8)$$

This is called the *weak form* of the boundary value problem and has the same solution as Eq. 2.1.

3.3 The Finite Element Approximation

Since Eq. 3.8 cannot be solved exactly for arbitrarily shaped domains and arbitrary boundary conditions, the weak form of the problem is solved approximately. Discretize the domain Ω so that the number of *finite elements* is NUMEL and the corresponding number of *nodal points* is NUMNP. Furthermore suppose that NEQ of the nodes correspond to locations where h is unknown (NEQ is an acronym for number of equations), hence (NUMNP-NEQ) nodes are on Γ_1. Then assume an approximate solution $\hat{h}$ as a linear combination of NUMNP functions defined over all of Ω:

$$h \cong \hat{h} = \sum_{j=1}^{NEQ} N_j(x,y) h_j(t) + \sum_{j=NEQ+1}^{NUMNP} N_j(x,y) g_j(t) \qquad (3.9)$$

where $N_j(x,y)$, $1 \le j \le$ NUMNP, is the jth interpolation function with value 1 at node j and value 0 at all other nodes,

$h_j(t)=h_j(x_j,y_j,t)$, $1 \le j \le$ NEQ, is the approximate value of h at node j at time t,

and $g_j(t) = h_1(x_j, y_j, t)$, $(NEQ+1) \leq j \leq NUMNP$, is the given or specified value of h at node j on Γ_1 at time t.

The notation here implies that the nodes have been numbered so that nodes on Γ_1 appear last, however, computationally this is not necessary.

Since h must satisfy Eq. 3.8 exactly, the approximation $\hat{h}$ is also forced to satisfy the equation. Whereas h satisfies Eq. 3.8 for all functions w which vanish on Γ_1, the unknown coefficients $h_j, j=1,\ldots,$ NEQ are chosen so that Eq. 3.8 is satisfied for each of NEQ chosen weighting functions, $w_i(x,y)$, $i=1,\ldots,NEQ$, which vanish on Γ_1. In this way NEQ equations are generated for the NEQ unknown nodal values h_j. It is clear that the accuracy of the approximate solution $\hat{h}$ depends very much on the particular choices of $N_j(x,y)$ and $w_i(x,y)$. Thus Eq. 3.10, below, represents a whole family of finite element methods where the N_j and w_i are chosen differently:

$$\int_\Omega [w_i S(\sum_1^{NEQ} N_j \frac{dh_j}{dt}) + \frac{\partial w_i}{\partial x} T_{xx}(\sum_1^{NEQ} \frac{\partial N_j}{\partial x} h_j) + \frac{\partial w_i}{\partial y} T_{yy}(\sum_1^{NEQ} \frac{\partial N_j}{\partial y} h_j)$$

$$+ w_i \frac{K'}{B'} (\sum_1^{NEQ} N_j h_j)]d\Omega + \int_{\Gamma_3} w_i \frac{K''W''}{B''} (\sum_1^{NEQ} N_j h_j) d\Gamma_3$$

$$= \int_{\Gamma_2} w_i Q_s d\Gamma_2 + \int_{\Gamma_3} w_i \frac{K''W''}{B''} h_3 d\Gamma_3 + \int_\Omega w_i (Q + \frac{K'}{B'} h_a) d\Omega$$

$$-\int_\Omega [w_i S(\sum_{NEQ+1}^{NUMNP} N_j \frac{dg_j}{dt}) + \frac{\partial w_i}{\partial x} T_{xx}(\sum_{NEQ+1}^{NUMNP} \frac{\partial N_j}{\partial x} g_j) + \frac{\partial w_i}{\partial y} T_{yy}(\sum_{NEQ+1}^{NUMNP} \frac{\partial N_j}{\partial y} g_j)$$

$$+ w_i \frac{K'}{B'} (\sum_{NEQ+1}^{NUMNP} N_j g_j)]d\Omega - \int_{\Gamma_3} w_i \frac{K''W''}{B''} (\sum_{NEQ+1}^{NUMNP} N_j g_j) d\Gamma_3 \qquad (3.10)$$

for $i = 1,\ldots,NEQ$,

where all summations are implicitly on j. This expression depends on the identities

$$\frac{\partial}{\partial t}\left[\sum_{1}^{NEQ} N_j h_j\right] = \sum_{1}^{NEQ} N_j \frac{dh_j}{dt}$$

$$\frac{\partial}{\partial x}\left[\sum_{1}^{NEQ} N_j h_j\right] = \sum_{1}^{NEQ} \frac{\partial N_j}{\partial x} h_j$$

and

$$\frac{\partial}{\partial y}\left[\sum_{1}^{NEQ} N_j h_j\right] = \sum_{1}^{NEQ} \frac{\partial N_j}{\partial y} h_j \quad .$$

Note that the last term in Eq. 3.10, an integral over Γ_3, should rigorously be zero since a node should not be on both Γ_1 and Γ_3. Loosely, however, it can be considered as a prescribed flux term which does not affect the solution, except for the flux at that node.

3.4 The Galerkin Finite Element Method

The Galerkin method is simply a method of choosing the weighting functions w_i in Eq. 3.10. According to this method the weighting functions are chosen to be the same as the interpolation functions, that is $w_i = N_i$. Notice that this choice of w_i satisfies the requirement $w = 0$ on Γ_1 since every N_i, $i = 1,\ldots,NEQ$ is zero at all nodes on Γ_1. The advantage of this particular choice of w_i is that the resulting set of NEQ equations can be represented in matrix form in terms of symmetric positive definite matrices, a feature not shared by all

other finite element methods. This results in the use of simpler computational methods for solving the equations. The result is still a whole family of methods, however, because the interpolation functions $N_i(x,y)$ are not yet defined.

3.5 The Matrix Form of the Equations

Substituting $w_i = N_i$ in Eq. 3.10 and rearranging the integrals and summations (since these are linear operations) gives

$$\sum_{j=1}^{NEQ} [\{\int_\Omega SN_iN_j d\Omega\} \frac{dh_j}{dt} + \{\int_\Omega (T_{xx} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + T_{yy} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y}$$

$$+ \frac{K'}{B'} N_iN_j)d\Omega + \int_{\Gamma_3} \frac{K''W''}{B''} N_iN_j d\Gamma_3\}h_j]$$

$$= \int_{\Gamma_2} N_iQ_s d\Gamma_2 + \int_{\Gamma_3} N_i \frac{K''W''}{B''} h_3 d\Gamma_3 + \int_\Omega N_i(Q + \frac{K'}{B'} h_a)d\Omega$$

$$- \sum_{j=NEQ+1}^{NUMNP} [\{\int_\Omega SN_iN_j d\Omega\} \frac{dg_j}{dt} + \{\int_\Omega (T_{xx} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + T_{yy} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y}$$

$$+ \frac{K'}{B'} N_iN_j)d\Omega + \int_{\Gamma_3} \frac{K''W''}{B''} N_iN_j d\Gamma_3\}g_j]$$

for $i = 1,\ldots,NEQ.$ (3.11)

This can be written in matrix form as

$$\underline{\underline{M}}\dot{\underline{h}} + \underline{\underline{K}}\underline{h} = \underline{f} - (\underline{\underline{M}}^*\dot{\underline{g}} + \underline{\underline{K}}^*\underline{g}) \tag{3.12}$$

in which the single underline (_) represents a vector and the double underline (=) represents a matrix, and where

$\underline{h} = \{h_j\}$, j=1,...,NEQ, a vector of unknown nodal values

$\dot{\underline{h}} = \frac{d}{dt}(\underline{h})$

$\underline{g} = \{g_j\}$, j=NEQ+1,...,NUMNP, a vector of known nodal values on Γ_1

$\dot{\underline{g}} = \frac{d}{dt}(\underline{g})$

$\underline{\underline{M}} = \{m_{ij}\}$, i=1,...,NEQ and j=1,...,NEQ

$\underline{\underline{K}} = \{k_{ij}\}$, i=1,...,NEQ and j=1,...,NEQ

$\underline{f} = \{f_i\}$, i=1,...,NEQ

$\underline{\underline{M}}^* = \{m_{ij}\}$ i=1,...,NEQ and j =NEQ+1,...,NUMNP

$\underline{\underline{K}}^* = \{k_{ij}\}$ i=1,...,NEQ and j =NEQ+1,...,NUMNP

$$m_{ij} = \int_\Omega SN_iN_j d\Omega \tag{3.12a}$$

$$k_{ij} = \int_\Omega (T_{xx} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + T_{yy} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} + \frac{K'}{B'} N_iN_j) d\Omega$$

$$+ \int_{\Gamma_3} \frac{K''W''}{B''} N_iN_j d\Gamma_3 \tag{3.12b}$$

and

$$f_i = \int_{\Gamma_2} N_iQ_s d\Gamma_2 + \int_{\Gamma_3} N_i \frac{K''W''}{B''} h_3 d\Gamma_3 + \int_\Omega N_i(Q + \frac{K'}{B'} h_a) d\Omega \tag{3.12c}$$

Eq. 3.12 represents a system of simultaneous ordinary differential equations in time for the unknown nodal values h_j, j=1,...,NEQ. It can be solved approximately at all the nodes in the finite element grid given

initial conditions (Eq. 2.5) and appropriate boundary conditions. For a steady state problem, Eq. 3.12 becomes

$$\underline{\underline{K}}\underline{h} = \underline{f} - \underline{\underline{K}}^{*}\underline{g} \tag{3.13}$$

which is solved for a given set of boundary conditions. A large part of the computational effort needed to solve Eqs. 3.12, 3.13 involves evaluating the integrals in Eqs. 3.12a,b,c. The complexity of the integrals depends on the type of interpolation functions used and on the spatial variation of aquifer properties and fluxes, etc., within element domains. It is often necessary to use numerical integration techniques.

The notation in Eq. 3.12 is largely influenced by structural engineering terminology. $\underline{\underline{M}}$, $\underline{\underline{K}}$ and $\underline{f}$ represent storage effects, internal conductivity effects and external fluxes respectively, and Eq. 3.12 (just like Eq. 2.1) is essentially a balance between change of storage, fluxes inside the aquifer and fluxes into or out of the aquifer. In structural engineering, an analogous equation to Eq. 3.12 represents a force balance on a structure, and $\underline{\underline{M}}$, $\underline{\underline{K}}$ and $\underline{f}$ represent mass (inertial), stiffness and force effects, respectively.

3.6 Interpolation Functions $N_i(x,y)$ and Their Properties

Up to this point the finite element solution has been defined in terms of an unspecified set of interpolation functions $N_i(x,y)$. Having adopted the Galerkin method, the accuracy of the approximate solution in space depends only on the choice of interpolation functions and the degree of discretization in the finite element mesh. In

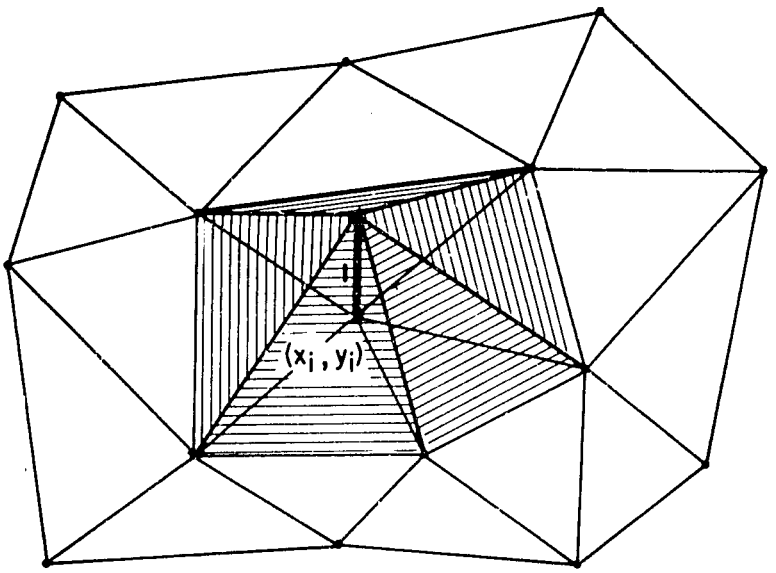
AQUIFEM-1 the simplest possible interpolation functions in two dimensions are chosen: these are called linear interpolation functions and the elements are thus known as linear triangular elements. As an example, an interpolation function at node i is shown in Figure 3.2. This figure also shows an approximation to a solution surface using finite elements of this type. It should be noted that interpolation functions can be thought of as *basis functions* which are described in standard texts on linear algebra.

In the derivation of the matrix form of the problem, Eq. 3.12, several integrals were defined over the aquifer domain and segments of the boundary. The matrices obtained are known as *global* matrices because of the global nature of these integrals over the whole domain Ω. It is convenient, however, to describe interpolation functions and their properties relative to the individual element domains, and this alternative viewpoint is also useful computationally. Notice that any integral can be written

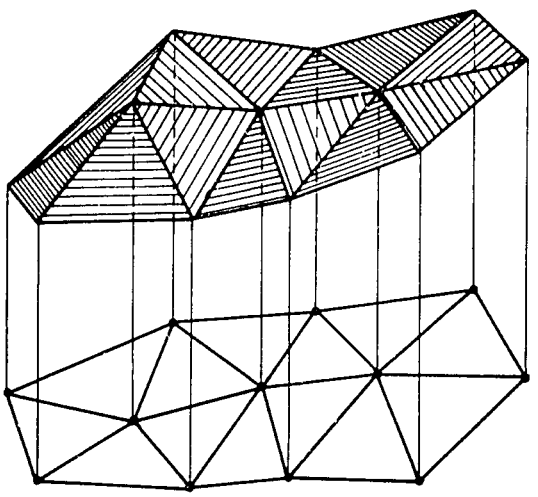
$$\int_{\Omega} F(x,y)d\Omega = \sum_{\ell=1}^{NUMEL} \left(\int_{\Omega_\ell^e} F(x,y)d\Omega_\ell^e\right) \tag{3.14}$$

where Ω_ℓ^e is the ℓth element domain and F is some function. Similar expressions can be written for boundary integrals.

From Figure 3.2 it is apparent that $N_i(x,y)$ is non-zero only within the elements which share node i as a common node. There are only three interpolation functions which are non-zero within the domain of any element Ω_ℓ^e: that is, the three interpolation functions defined



a) Linear interpolation function $N_i(x,y)$ is a pyramid centered at node i with zero values outside the elements which share node i



b) Approximation to a solution surface consists of a mosaic of triangular segments of plane surfaces

Figure 3.2 Linear Interpolation Functions.

for the nodes of that element. If the nodes in each element are renumbered 1, 2 and 3 in a *local* node numbering scheme, the three interpolation functions associated with any linear triangular element are as are shown in Figure 3.3.

The function h(x,y) is then approximated over the element domain by

$$\hat{h}(x,y) = \sum_{i=1}^{3} N_i h_i = N_1 h_1 + N_2 h_2 + N_3 h_3 \tag{3.15}$$

where h_1, h_2, h_3 are the nodal values of $\hat{h}$. That is, the function h is approximated over Ω^e by a plane which passes through the three nodal values of $\hat{h}$. In vector form Eq. 3.15 becomes

$$\hat{h}(x,y) = [N_1 \; N_2 \; N_3] \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} = \underline{N}^T \underline{h} \tag{3.16}$$

where the superscript $(\;)^T$ indicates a vector transpose. An alternative representation of a plane (from Cartesian geometry) is

$$\begin{aligned} \hat{h}(x,y) &= \alpha_1 + \alpha_2 x + \alpha_3 y \\ &= [1 \; x \; y] \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} \\ &= \underline{p}^T \underline{\alpha} \end{aligned} \tag{3.17}$$

But the plane passes through the values h_1, h_2 and h_3 at the nodes, thus

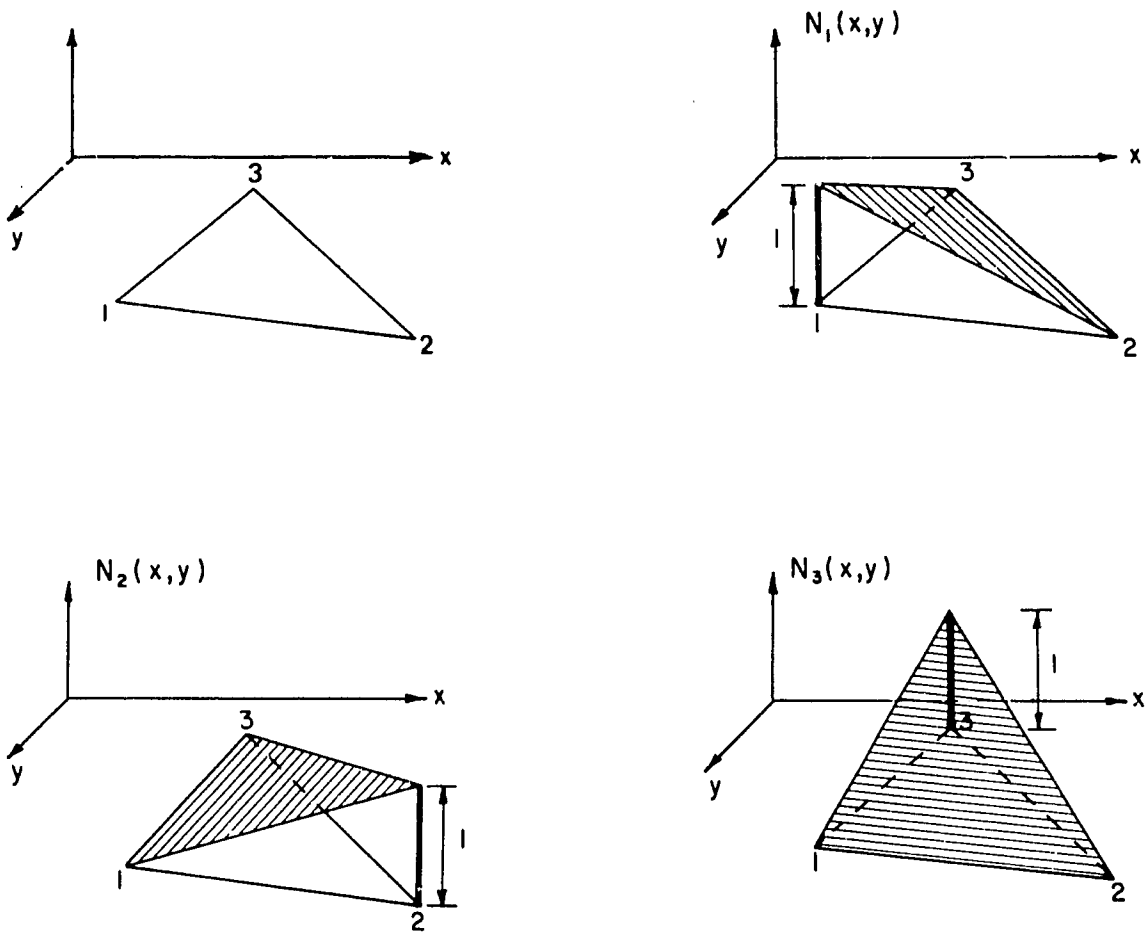


Figure 3.3 Finite Element and Element Interpolation Functions.

$$\hat{h}(x_1,y_1) = h_1 = \alpha_1 + \alpha_2 x_1 + \alpha_3 y_1$$

$$\hat{h}(x_1,y_2) = h_2 = \alpha_1 + \alpha_2 x_2 + \alpha_3 y_2$$

$$\hat{h}(x_3,y_3) = h_3 = \alpha_1 + \alpha_2 x_3 + \alpha_3 v_3$$

or $\quad \underline{h} = \underline{\underline{G}}\ \underline{\alpha} \qquad (3.18)$

where $\quad \underline{\underline{G}} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix}$

Solving Eq. 3.18 for $\underline{\alpha}$ and substituting in Eq. 3.17,

$$\hat{h}(x,y) = \underline{p}^T\ \underline{\underline{G}}^{-1}\ \underline{h} \qquad (3.19)$$

which by comparison with Eq. 3.16 leads to

$$\underline{N}^T = \underline{p}^T\ \underline{\underline{G}}^{-1} \qquad (3.20)$$

It is relatively simple to invert the matrix $\underline{\underline{G}}$ to obtain (Zienkiewicz, 1977)

$$N_1(x,y) = \frac{1}{2A}(a_1 x + b_1 y + c_1) \quad \text{where} \quad \begin{aligned} a_1 &= y_2 - y_3 \\ b_1 &= x_3 - x_2 \\ c_1 &= x_2 y_3 - x_3 y_2 \end{aligned}$$

$$N_2(x,y) = \frac{1}{2A}(a_2 x + b_2 y + c_2) \quad \text{where} \quad \begin{aligned} a_2 &= y_3 - y_1 \\ b_2 &= x_1 - x_3 \\ c_2 &= x_3 y_1 - x_1 y_3 \end{aligned} \qquad (3.21)$$

$$N_3(x,y) = \frac{1}{2A}(a_3 x + b_3 y + c_3) \quad \text{where} \quad \begin{aligned} a_3 &= y_1 - y_2 \\ b_3 &= x_2 - x_1 \\ c_3 &= x_1 y_2 - x_2 y_1 \end{aligned}$$

where $A = \frac{1}{2}|\underline{\underline{G}}| = 1/2$ the determinant of $\underline{\underline{G}}$ is the area of the element. For A to be positive, the three nodes must be given in a counterclockwise direction around the element.

Now recall from the matrix form of the equations (Eq. 3.12) that some assumption is needed about the variation of quantities such as S, T_{xx}, T_{yy}, K'/B', etc., over each element domain, Ω^e, or boundary segment, Γ^e. In AQUIFEM-1, all such quantities are assumed to be approximately constant over each element domain, hence it is only necessary to evaluate

$$\int_{\Omega^e} N_i N_j d\Omega^e, \int_{\Omega^e} \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} d\Omega^e, \int_{\Omega^e} \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} d\Omega^e,$$

$$\int_{\Omega^e} N_i d\Omega^e, \int_{\Gamma^e} N_i N_j d\Gamma^e \text{ and } \int_{\Gamma^e} N_i d\Gamma^e .$$

It can be shown (e.g., Eisenberg and Malvern, 1973) that for linear triangular elements, if $i,j,k \in \{1,2,3\}$, then

$$\int_{\Omega^e} N_i^p N_j^q N_k^r d\Omega^e = \frac{p!q!r!}{(p+q+r+2)!} 2A \tag{3.22a}$$

$$\int_{\Gamma^e} N_i^p N_j^q \, d\Gamma^e = \frac{p!q!}{(p+q+1)!} s \tag{3.22b}$$

where s is the length of an element side. Furthermore from Eq. 3.21, it is clear that

$$\frac{\partial N_i}{\partial x} = \frac{1}{2A} a_i \tag{3.23a}$$

$$\frac{\partial N_i}{\partial y} = \frac{1}{2A} b_i \tag{3.23b}$$

which are constant over the element domain. The availability of these analytical expressions is one of the greatest attractions of triangular elements, since numerical spatial integration is completely avoided. It is thus possible to simplify all of the integrals required for the matrix equations:

$$\int_{\Omega^e} N_i N_j d\Omega^e = \begin{cases} \frac{A}{12} \text{ for } i \neq j \\ \frac{A}{6} \text{ for } i = j \end{cases} \tag{3.24a}$$

$$\int_{\Omega^e} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} d\Omega^e = \frac{a_i a_j}{4A} \tag{3.24b}$$

$$\int_{\Omega^e} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} d\Omega^e = \frac{b_i b_j}{4A} \tag{3.24c}$$

$$\int_{\Omega^e} N_i d\Omega^e = A/3 \tag{3.24d}$$

$$\int_{\Gamma^e} N_i N_j \, d\Gamma^e = \begin{cases} s/6 \text{ for } i \neq j \\ s/3 \text{ for } i = j \end{cases} \tag{3.24e}$$

$$\int_{\Gamma^e} N_i \, d\Gamma^e = s/2 \tag{3.24f}$$

3.7 Assembly of the Matrices

The final step in setting up the matrix problem involves relating the terms obtained as element integrals to the terms of the global

matrices. Define element matrices corresponding to the global matrices by:

$$\underline{\underline{m}}^e = \{m_{ij}\},\ i,j = 1,\ldots,3$$

$$\underline{\underline{k}}^e = \{k_{ij}\},\ i,j = 1,\ldots,3 \qquad (3.25)$$

$$\underline{f}^e = \{f_i\},\ \ i = 1,\ldots,3$$

where m_{ij}, k_{ij} and f_i are as defined in Eqs. 3.12a,b,c but with integrals over the element domain, Ω^e, or element boundary, Γ^e. It is then possible to explicitly obtain all of these matrices using the results given in Eq. 3.24.

If storativity S is assumed constant over the element domain, then

$$\underline{\underline{m}}^e = S\,\frac{A}{12}\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \qquad (3.26)$$

Similarly, if transmissivities T_{xx}, T_{yy} and leakage properties K'/B' are approximately constant over the element, then

$$\underline{\underline{k}}^e = \frac{1}{4A}\left\{ T_{xx}\begin{bmatrix} a_1^2 & a_1a_2 & a_1a_3 \\ a_2a_1 & a_2^2 & a_2a_3 \\ a_3a_1 & a_3a_2 & a_3^2 \end{bmatrix} + T_{yy}\begin{bmatrix} b_1^2 & b_1b_2 & b_1b_3 \\ b_2b_1 & b_2^2 & b_2b_3 \\ b_3b_1 & b_3b_2 & b_3^2 \end{bmatrix}\right\}$$

$$+ \frac{K'}{B'}\,\frac{A}{12}\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} + \text{other terms, if any element sides are on } \Gamma_3 \qquad (3.27)$$

The terms due to Γ_3 are difficult to express mathematically. However, the use of an *assembly operator* allows an understanding of how these terms are added in.

First consider the terms generated by a single side of an element. Let the nodes on a side be once more renumbered 1 and 2 (independent of the local element node numbers or the global node numbers). Then if K"W"/B" is constant on an element side of Γ_3, Eqs. 3.12b and 3.24 define the additional terms in Eq. 3.27 as

$$\int_{\Gamma_3} \frac{K''W''}{B''} N_i N_j d\Gamma_3 = \begin{cases} w_3 \dfrac{K''W''}{B''} \dfrac{s}{6} & \text{for } i \neq j \\ w_3 \dfrac{K''W''}{B''} \dfrac{s}{3} & \text{for } i = j \end{cases} \tag{3.28}$$

for i, j = 1, 2

where w_3 is a weighting factor, equal to the inverse of the number of elements (either one or two) which share the side in question. Defining $\underline{\underline{k}}_3$ as a *contribution* to $\underline{\underline{k}}^e$ due to a side on Γ_3, then

$$\underline{\underline{k}}_3 = w_3 \frac{K''W''}{B''} \frac{s}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \tag{3.29}$$

Finally define the element *assembly operator* $\underset{\sigma=1}{\overset{3}{A}}(\ \ )$ which loops over the 3 sides of an element and performs a mapping between side node numbers and element node numbers if the side is on Γ_3. That is, it adds $\underline{\underline{k}}_3$ into the right places in $\underline{\underline{k}}^e$ for each side on Γ_3. For example, if the side connecting element nodes 1 and 3 is on Γ_3, the four terms in Eq. 3.29 are added appropriately to k^e_{11}, k^e_{13}, k^e_{31} and k^e_{33} in $\underline{\underline{k}}^e$. Thus using the notation defined here, the additional terms in Eq. 3.27 can be written:

$$\mathop{A}_{\sigma=1}^{3} \left[w_3\left(\frac{K''W''}{B''}\right) \frac{s}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}\right] \tag{3.30}$$

The terms in the element *flow* vector $\underline{f}^e$ are more difficult to express than $\underline{k}^e$. This is partly because more assembly operations are needed for integrals along Γ_2 and Γ_3 (see Eq. 3.12c), but also because until now the source/sink term $Q = Q(x,y,t)$ has not been discussed in detail. In groundwater applications Q represents either a distributed or a point inflow or outflow. It makes sense therefore to allow two expressions for the effect of these different kinds of fluxes on the vector $\underline{f}^e$: Q_n $[L^3/T]$ is defined as a point inflow at a single node and Q_e $[L/T]$ is defined as a uniform distributed inflow over the element area. Assuming that $Q_s[L^2/T]$ is a uniform inflow along a side on Γ_2, that $(K''B''/W'')$ is constant along a side on Γ_3, and that (K'/B') is constant over the element, then

$$\underline{f}^e = \frac{A}{3} Q_e \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + \frac{A}{12} \frac{K'}{B'} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \begin{bmatrix} h_{a,1} \\ h_{a,2} \\ h_{a,3} \end{bmatrix} + \mathop{A}_{\nu=1}^{3} (w_n Q_n)$$

$$+ \mathop{A}_{\sigma=1}^{3} \left(w_2 Q_s \frac{s}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix}\right) + \mathop{A}_{\sigma=1}^{3} \left(w_3 \frac{K''W''}{B''} \frac{s}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} h_{3,1} \\ h_{3,2} \end{bmatrix}\right) \tag{3.31}$$

where $h_{a,1}$, $h_{a,2}$ and $h_{a,3}$ are heads in an adjacent leaky layer given as nodal values; w_n is a weighting factor, equal to the inverse of the number of elements sharing a given node; w_2 is a weighting factor, equal to the inverse of the number of elements sharing a side on Γ_2; and $h_{3,1}$ and $h_{3,2}$ are the 3rd-type boundary heads at the ends of the particular element side. Here there are three different assembly operators which loop

over element nodes or element sides and add contributions to the vector $\underline{f}^e$ as required.

Given element matrices as defined by Eqs. 3.25, it remains to be shown how the global matrices $\underline{\underline{M}}$ and $\underline{\underline{K}}$, and global flux vector $\underline{f}$ are formed. Using the concept of an assembly operator again, define a global operator which loops over all the elements in the finite element grid, and adds the terms of the element matrices into the global matrices. This operator maps the local element node numbers into the global node numbers for each element. Thus

$$\underline{\underline{M}} = \mathop{A}_{\ell=1}^{NUMEL} (\underline{\underline{m}}_\ell^e)$$

$$\underline{\underline{K}} = \mathop{A}_{\ell=1}^{NUMEL} (\underline{\underline{k}}_\ell^e) \qquad (3.32)$$

$$\underline{f} = \mathop{A}_{\ell=1}^{NUMEL} (\underline{f}_\ell^e)$$

where terms from the element matrices are only added in if the nodes are not on Γ_1, (in accordance with the ranges i,j = 1,...,NEQ given after Eq. 3.12). With similar definitions applying to $\underline{\underline{M}}^*$ and $\underline{\underline{K}}^*$, it is now possible to define all the terms in the matrix equation, Eq. 3.12, in terms of element geometry (A, s, a_i, b_i, etc.), element aquifer properties (S, T_{xx}, T_{yy}, $\frac{K'}{B'}$, etc.) and boundary conditions (known heads g, Q_s, $\frac{K''W''}{B''}$, etc.). The only remaining question is how to solve Eq. 3.12 in time. This question is discussed in Chapter 4 after a brief summary of the convergence properties of the finite element method in space, and a discussion of modifications to the solution procedure which are employed by AQUIFEM-1.

3.8 Convergence of the Finite Element Method

It is useful at this stage to discuss the accuracy of the procedures described in Section 3.3 for approximating the spatial variation of the piezometric head. It was mentioned in Section 3.1 that interpolation functions cannot be chosen completely arbitrarily. In fact it can be shown (Zienkiewicz, 1977) that the interpolation functions (and hence the approximate solution $\hat{h}(x,y,t)$) must satisfy the following conditions:

1) The interpolation function must be smooth inside all elements (smoothness requirement).
2) The interpolation function and all its derivatives up to order one less than the highest derivative of h in the weak form (say order m-1 where m = 1 for Eq. 3.8), must be continuous at boundaries between elements (compatibility requirement).
3) In the limit, when the element size shrinks to zero, derivatives of order m must be constant within the element (completeness requirement).

Although in certain circumstances the first two conditions may be relaxed, the linear triangular elements used in AQUIFEM-1 satisfy all three requirements when m = 1. This kind of element belongs to a family of *isoparametric* elements which shares these properties.

It is possible to say a little more about the convergence of the method. Let $\underline{h}$ be the vector of nodal values computed using the Galerkin finite element method and let $\underline{h}^*$ be a vector containing the exact solutions at those nodes. Then the method is said to be convergent if the error in the approximate solution satisfies

$$\|\underline{e}\| = \|\underline{h}^* - \underline{h}\| \leq C\, r^u \tag{3.33}$$

where $\| \ \|$ represents a *norm* of the vector, which measures its length in some sense,

C is constant for a particular problem (depending on geometry, material properties and the exact solution),

r is a length which characterizes the degree of discretization (i.e., the size of the elements),

and $u > 0$ is the rate of convergence.

It can be shown (Strang and Fix, 1973) that for the groundwater flow equation (where the highest spatial derivative of h in the weak form, Eq. 3.8, is of order $m = 1$) and for linear interpolation functions (which can exactly represent polynomials up to degree $k = 1$), the rate of convergence is given by

$$u = k + m = 2.$$

That is, if the element size were halved, the error in the approximate solution would decrease by a factor of four. A similar expression to Eq. 3.33 can be obtained for the error in the derivatives of the piezometric head. In particular for the method used in AQUIFEM-1, the derivatives are first order convergent. It is apparent that decreasing the element size significantly improves the approximate solution, and that solutions with different degrees of discretization would allow an estimate of the error in the solution. Unfortunately, however, discretization is usually controlled by economic constraints.

Convergence criteria are widely discussed in the literature. For more details the reader is advised to see Strang and Fix (1973), Zienkiewicz (1977), Huebner (1975) or Pinder and Gray (1977).

3.9 Modifications of the General Procedure

The various equations in Section 3.7 which define the element matrices $\underline{\underline{m}}^e$, $\underline{\underline{k}}^e$ and $\underline{f}^e$ are rigorous applications of the Galerkin procedure under the assumptions stated in that section. These were assumptions involving the constancy of many parameters over element domains or along element sides. However, in groundwater analysis, given the long characteristic response times and very gradual spatial changes in piezometric head, the approximations are believed to be adequate. The purpose of this section is to describe a few modifications to the rigorous procedure which greatly simplify implementation in AQUIFEM-1 and which are still believed to be reasonable approximations.

It is common practice in the dynamic analysis of structures or fluids to use a technique called *mass lumping* to diagonalize the *storage* matrix $\underline{\underline{M}}$. This is very advantageous when *explicit* methods are used to solve the matrix equations in time with very short time steps. Although explicit methods are not used in AQUIFEM-1, a type of mass lumping was found to be useful for treating the storativity matrix $\underline{\underline{M}}$. There are many types of mass lumping which can be described theoretically by numerical integration rules for performing the integral in Eq. 3.12a. In practice, however, all procedures for linear triangular elements are equivalent to adding the values in each row of $\underline{\underline{m}}^e$ and placing the result on the diagonal. Thus a lumped storage matrix can be written

$$\underline{\underline{m}}^e = S \frac{A}{3} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{3.34}$$

where S is constant over the element. Since it is possible in some cases for part of an element to be confined and the remaining part to be phreatic, a constant value of S over a whole element seems inappropriate, especially since heads are only computed at the nodes. For this reason the element storage matrix is further modified in AQUIFEM-1, so that

$$\underline{\underline{m}}^{e}_{\text{AQUIFEM-1}} = \frac{A}{3}\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_2 & 0 \\ 0 & 0 & S_3 \end{bmatrix} \tag{3.35}$$

where S_j, $j=1,\ldots,3$ are heuristically determined depending on whether or not the status changes at one of the three nodes during a given time step. At the start of a time step S_j is either S_oB or S_y depending on the status at the jth element node. If the status of the jth node changes during the time step, $S_j^{(i+1)}$ at the (i+1)th iteration* is given by:

$$S_j^{(i+1)} = 0.7S_j^{(i)} + 0.3\ \frac{[(h_n-(z+B))S_oB + (z+B-h_{n+1}^{(i)})S_y]}{(h_n-h_{n+1}^{(i)})} \tag{3.36}$$

where h_n is the head at end of the previous time step and $h_{n+1}^{(i)}$ is the approximate head for this time step after the previous iteration. The term in brackets is based on an argument of local conservation of mass during the given time step and is also used by Prickett and Lonnquist (1971) and Trescott et al. (1976). The weighting coefficients of 0.7 for the previous time step and 0.3 for the current time step are empirical factors observed to produce best results.

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*Iterative methods of solution of the matrix equation are described in Chapter 4.

Approximations analogous to mass lumping have been made in other matrices to reduce storage and save computation time. In particular,

$$\underline{k}^e_{\text{AQUIFEM-1}} = \frac{1}{4A}\left\{ T_{xx}\begin{bmatrix} a_1^2 & a_1a_2 & a_1a_3 \\ a_2a_1 & a_2^2 & a_2a_3 \\ a_3a_1 & a_3a_2 & a_3^2 \end{bmatrix} + T_{yy}\begin{bmatrix} b_1^2 & b_1b_2 & b_1b_3 \\ b_2b_1 & b_2^2 & b_2b_3 \\ b_3b_1 & b_3b_2 & b_3^2 \end{bmatrix}\right\}$$

$$+ \frac{K'}{B'}\frac{A}{3}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \mathop{A}_{\sigma=1}^{3} \left[w_3\left(\frac{K''W''}{B''}\right)\frac{s}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right] \qquad (3.37)$$

$$\underline{f}^e_{\text{AQUIFEM-1}} = \frac{A}{3} Q_e \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + \frac{A}{3}\frac{K'}{B'}\begin{bmatrix} h_{a,1} \\ h_{a,2} \\ h_{a,3} \end{bmatrix} + \mathop{A}_{\nu=1}^{3} (w_n Q_n)$$

$$+ \mathop{A}_{\sigma=1}^{3} \left(w_2 Q_s \frac{s}{2}\begin{bmatrix} 1 \\ 1 \end{bmatrix}\right) + \mathop{A}_{\sigma=1}^{3} \left[w_3\left(\frac{K''W''}{B''}\right)\frac{s}{2}\begin{bmatrix} h_{3,1} \\ h_{3,2} \end{bmatrix}\right] \qquad (3.38)$$

Although the procedures described here may seem arbitrary, they have been shown to work adequately and they certainly result in smaller computational effort.

As a final note on approximations in AQUIFEM-1, the computation of element properties S, T_{xx}, T_{yy}, $\frac{K'}{B'}$, etc., should be discussed. AQUIFEM-1 has many input options for the convenience of the user. For example properties may be input for individual elements or for individual nodes. In either case some quantities need to be converted to the other form because of the way they are used in the element matrices.

This conversion is performed by areal-weighted averaging. If nodal quantities are input, the use of averaged transmissivities $\overline{T}_{xx}$ and $\overline{T}_{yy}$ in Eq. 3.36 can be shown to be exactly equivalent to integrating a linear variation in these properties over the elements. The conversion of element storativities to lumped nodal storativities is not believed to be a poor approximation because of the inherent uncertainties in these parameters. Similar comments apply to all other quantities since they are in practice very hard to estimate. Indeed it is common in groundwater models to allocate the same aquifer properties to large areas (represented by many elements) since it is not possible to distinguish parameters on a finer scale because of small amounts of available data. In such cases the averaging described above has little effect.

Chapter 4

SOLUTION OF THE MATRIX EQUATIONS

4.1 General Considerations

The final matrix equation (Eq. 3.12) obtained in Section 3.5 constitutes a system of ordinary differential equations in time. Several numerical schemes are available to perform time integration of this equation. Of these, AQUIFEM-1 employs a finite difference method which uses the distribution of heads at time t to compute the heads at $t + \Delta t$.

Practical groundwater problems can be classified as steady or unsteady depending on whether or not heads and boundary conditions change with time. If $\partial h/\partial t = 0$ in Eq. 2.1, the problem is steady and a knowledge of the storativity S is not required. In this case the matrix problem is easily solved without a time integration scheme.

Another useful classification depends on whether or not transmissivities depend on the piezometric head. Since transmissivity is defined as the product of hydraulic conductivity and the saturated thickness, it follows that the transmissivities of confined aquifers are independent of head (which is usually denoted ϕ in this case), whereas the transmissivities of unconfined or phreatic aquifers vary with head. In the first case the matrix $\underline{\underline{K}}$ is constant in time and Eq. 3.12 is linear in $\underline{h}$, while in the second case $\underline{\underline{K}} = \underline{\underline{K}}(\underline{h})$ depends on the solution itself and Eq. 3.12 is nonlinear. The terms linear and confined are used synonomously with regard to AQUIFEM-1. Similarly,

the terms nonlinear, unconfined and phreatic are interchangeable. When solving nonlinear problems, an iterative method is needed because the transmissivities are not known in advance. In some cases, for example when an aquifer changes from being phreatic to confined during a time step, the storativities may not be known in advance and $\underline{\underline{M}} = \underline{\underline{M}}(\underline{h})$ causes further complications.

4.2 Steady State Problems

If $\partial h/\partial t = 0$, Eq. 3.12 reduces to Eq. 3.13:

$$\underline{\underline{K}}\,\underline{h} = \underline{f} - \underline{\underline{K}}^{*}\underline{g} \tag{4.1}$$

This equation is a simple set of NEQ simultaneous algebraic equations. The right-hand side includes contributions from fluxes through 2nd- and 3rd-type boundaries, distributed or point sources or sinks, and leakage fluxes (all of which are in $\underline{f}$), plus contributions due to the known head values $\underline{g}$.

If the aquifer is linear, AQUIFEM-1 uses a special equation solver which takes advantage of the symmetric profile structure of $\underline{\underline{K}}$ to solve Eq. 4.1 directly for $\underline{h}$. If the aquifer is nonlinear, an iterative technique is used as follows. Let $\underline{\underline{K}}^{(i)}$ be evaluated using transmissivities which depend on $\underline{h}^{(i)}$, the approximate solution at the ith iteration. Then the next approximation $\underline{h}^{(i+1)}$ can be obtained by *fixed-point* iteration (Conte and de Boor, 1972)

$$\underline{\underline{K}}^{(i)}\underline{h}^{(i+1)} = \underline{f} - \underline{\underline{K}}^{*(i)}\underline{g} \tag{4.2}$$

Subtracting $\underline{\underline{K}}^{(i)}\underline{h}^{(i)}$ from each side and denoting $\underline{h}^{(i+1)}-\underline{h}^{(i)}$ by $\underline{\Delta h}^{(i+1)}$ yields,

$$\underline{\underline{K}}^{(i)}\underline{\Delta h}^{(i+1)} = \underline{f} - \underline{\underline{K}}^{*(i)}\underline{g} - \underline{\underline{K}}^{(i)}\underline{h}^{(i)} \tag{4.3}$$

This procedure is continued until $\underline{\Delta h}^{(i+1)}$ becomes acceptably small, as defined by some *norm* of this vector. As $\underline{\Delta h}^{(i+1)}$ tends to zero, the left-hand side approaches zero and $\underline{h}^{(i)}$ is the desired approximate solution. Although Eqs. 4.2 and 4.3 give the same result at every iteration, Eq. 4.3 is utilized in AQUIFEM-1 since it has been found that acceptable convergence is obtained without updating $\underline{\underline{K}}^{(i)}$ on the <u>left</u>-hand side at every iteration. This may result in decreased computational effort since *factoring* the left-hand side matrix is a significant part of the total cost of a nonlinear simulation.

At present two different kinds of convergence criteria are used in AQUIFEM-1. One norm of the vector $\underline{h}^{(i+1)}$ is the root mean square error:

$$\sqrt{\sum_{j=1}^{NEQ} (\Delta h_j^{(i+1)})^2 / NEQ} \tag{4.4}$$

A second norm is simply the maximum absolute difference between iterations at any node point:

$$\max_{j=1,\ldots,NEQ} \left| \Delta h_j^{(i+1)} \right| \tag{4.5}$$

In some sense these norms (or measures of the *size* of the vector $\underline{\Delta h}$)

are equivalent. Iteration is stopped when the norm of $\underline{\Delta h}$ is smaller than some specified amount, or when a maximum number of iterations is exceeded.

4.3 Unsteady, Transient Problems

For non-steady situations, Eq. 3.12 is solved in time, given initial conditions $\underline{h}(t_0)$ at time t_0, and boundary conditions that can be time varying. A relatively common finite-difference method is used to solve these equations: in fact it is a family of generalized trapezoidal methods (see for example Hughes, 1977) of which forward and backward differences and the trapezoidal rule are special cases.

To motivate the notation to be used here, it is instructive to consider a simple ordinary differential equation in only one unknown which has a structure similar to Eq. 3.12:

$$\dot{h} + \lambda h = v + \lambda h = 0 \tag{4.6}$$

where $\dot{h}$ represents the time derivative of h(t) and v is introduced for notational purposes only. If the initial condition $h(t_0) = h_0$ is known at time t_0, the exact solution of this equation is

$$h = h_0 e^{-\lambda t} \quad . \tag{4.7}$$

Similarly, given $h(t_n)$ at time t_n, the exact solution at time $t_{n+1} = t_n + \Delta t$ is

$$h(t_{n+1}) = h(t_n)e^{-\lambda \Delta t} \tag{4.8}$$

In attempting to solve Eq. 4.6 numerically using discrete time steps, any procedure essentially tries to mimic the exponential behavior of Eq. 4.8.

Suppose the *approximate* solution is known at time t_n and that it satisfies Eq. 4.6 at that time:

$$v_n + \lambda h_n = 0 \tag{4.9}$$

where v_n, h_n are now approximations to the exact solution $v(t_n)$, $h(t_n)$. It is then necessary for the approximate solution at time t_{n+1} to satisfy

$$v_{n+1} + \lambda h_{n+1} = 0 \quad . \tag{4.10}$$

Now a common approximation for v_n using finite differences is the *forward difference* expression

$$v_n = \left.\frac{dh}{dt}\right|_n = \frac{h_{n+1}-h_n}{\Delta t} \quad , \tag{4.11}$$

so-called because it uses information at a later time to approximate the derivative. Another approximation is the *backward difference* expression

$$v_{n+1} = \left.\frac{dh}{dt}\right|_{n+1} = \frac{h_{n+1}-h_n}{\Delta t} \tag{4.12}$$

which uses information at a previous time. The most general approximation of this type is the weighted average

$$v_{n+\alpha} = (1-\alpha)v_n + \alpha v_{n+1} = \frac{h_{n+1}-h_n}{\Delta t} \tag{4.13}$$

where $0 \leq \alpha \leq 1$ is a weighting coefficient. Figure 4.1 shows how this family of methods predicts different values of h_{n+1} depending on the value of α. Note that $\alpha = 0$ corresponds to forward differences, often called the *explicit* method, because h_{n+1} can be explicitly evaluated using information already available, and that $\alpha = 1$ is the backward difference or *fully implicit* method, since in general v_{n+1} is not known until h_{n+1} is known and it is necessary to solve simultaneous equations for multi-dimensional problems. All methods with $0 < \alpha < 1$ are also called implicit methods. The special case $\alpha = 0.5$ is called the trapezoidal rule or the Crank-Nicolson method and has special properties in terms of accuracy of the approximation. Multiplying Eq. 4.9 by $(1-\alpha)$, Eq. 4.10 by α, adding the results and substituting Eq. 4.13 gives:

$$\frac{h_{n+1}-h_n}{\Delta t} + \lambda(\alpha h_{n+1} + (1-\alpha)h_n) = 0 \tag{4.14}$$

which can be solved for h_{n+1} given h_n. Rearranging terms yields

$$h_{n+1} = \frac{1-(1-\alpha)\Delta t\lambda}{1 + \alpha\Delta t\lambda} \; h_n \tag{4.15}$$

which is the discrete approximation to Eq. 4.8.

Before discussing matters of accuracy, stability and convergence, the methods above can be generalized to the groundwater problems described by Eq. 3.12. It can be shown using techniques of linear algebra (involving the generalized eigenvlaue problem associated with Eq. 3.12), that Eq. 3.12 can be equivalently represented by a

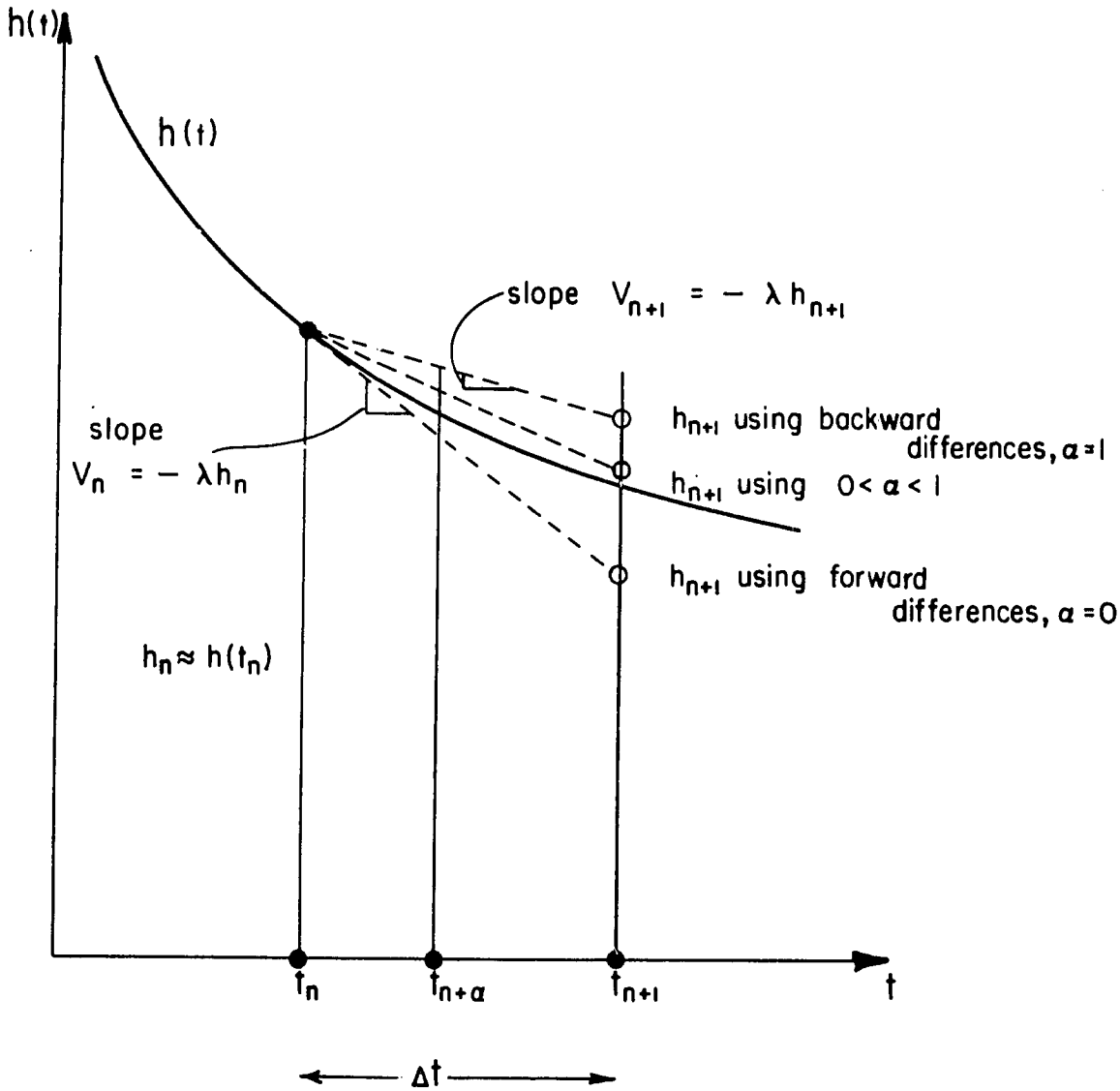

Figure 4.1 Finite Difference Temporal Approximations.

set of NEQ independent *decoupled* equations which can each be solved using the simple method described. At the outset, note that the aim is to solve Eq. 3.12 at time t_{n+1} as accurately as possible, given the approximate solution at t_n. Thus if $\underline{h}_{n+1}$, $\underline{v}_{n+1}$ are approximations of $\underline{h}(t_{n+1})$, $\dot{\underline{h}}(t_{n+1})$, respectively, Eq. 3.12 can be rewritten:

$$\underline{\underline{M}}_{n+1}\underline{v}_{n+1} + \underline{\underline{K}}_{n+1}\,\underline{h}_{n+1} = \underline{f}_{n+1} - \underline{\underline{M}}^{*}_{n+1}\,\dot{\underline{g}}_{n+1} - \underline{\underline{K}}^{*}_{n+1}\,\underline{g}_{n+1} \tag{4.16}$$

where the approximation $\underline{v}_{n+1}$ is discussed below. Suppose, by analogy with Eq. 4.13, that

$$\begin{aligned} \underline{h}_{n+1} &= \underline{h}_n + \Delta t((1-\alpha)\underline{v}_n + \alpha\underline{v}_{n+1}) \\ &= \underline{h}_n + \Delta t\,\underline{v}_{n+\alpha} \\ &= \tilde{\underline{h}}_{n+1} + \alpha\Delta t\underline{v}_{n+1} \end{aligned} \tag{4.17}$$

where $\tilde{\underline{h}}_{n+1} = \underline{h}_n + (1-\alpha)\Delta t\underline{v}_n$ is known at the start of the new time step. The vector $\tilde{\underline{h}}_{n+1}$ is loosely referred to as a *predictor* of the new vector $\underline{h}_{n+1}$, and $\underline{v}_{n+1}$ is thus defined in terms of $\underline{h}_{n+1}$ and $\tilde{\underline{h}}_{n+1}$. Substituting $\underline{v}_{n+1}$ from Eq. 4.17 into Eq. 4.16 and rearranging:

$$\begin{aligned} \left(\frac{1}{\alpha\Delta t}\,\underline{\underline{M}}_{n+1} + \underline{\underline{K}}_{n+1}\right)\underline{h}_{n+1} &= \underline{f}_{n+1} - \underline{\underline{M}}^{*}_{n+1}\,\dot{\underline{g}}_{n+1} \\ &\quad - \underline{\underline{K}}^{*}_{n+1}\,\underline{g}_{n+1} + \frac{1}{\alpha\Delta t}\,\underline{\underline{M}}_{n+1}\,\tilde{\underline{h}}_{n+1} \end{aligned} \tag{4.18}$$

This is the set of equations which is solved at each time step in AQUIFEM-1. Note, however, that the explicit method ($\alpha = 0$) is not

possible in this form. To implement the explicit method, set α equal to zero in Eq. 4.17, solve for $\underline{h}_{n+1}$, and then solve Eq. 4.16 for $\underline{v}_{n+1}$.

For linear problems, with constant time steps, the matrix $(\frac{1}{\alpha\Delta t}\underline{\underline{M}} + \underline{\underline{K}})$, which is referred to as the *system* matrix, is constant for all time steps. The matrix need only be *factored* once and the system is easily solved in time. It is sometimes desirable to vary the time step because the effect of changes in boundary conditions is rapid near the time of the change, but much slower at large times. In this case the system matrix must be reformed and factored whenever Δt changes.

For nonlinear problems, the solution of Eq. 4.18 is the same as a nonlinear steady state problem at every time step. Again fixed point iteration is used to give

$$(\frac{1}{\alpha\Delta t}\underline{\underline{M}}_{n+1}^{(i)} + \underline{\underline{K}}_{n+1}^{(i)})\underline{\Delta h}^{(i+1)} = \underline{f}_{n+1} - \underline{\underline{M}}_{n+1}^{*(i)}\dot{\underline{g}}_{n+1} - \underline{\underline{K}}_{n+1}^{*(i)}\underline{g}_{n+1}$$

$$+ \frac{1}{\alpha\Delta t}\underline{\underline{M}}_{n+1}^{(i)}\tilde{\underline{h}}_{n+1} - (\frac{1}{\alpha\Delta t}\underline{\underline{M}}_{n+1}^{(i)} + \underline{\underline{K}}_{n+1}^{(i)})\underline{h}_{n+1}^{(i)} \qquad (4.19)$$

Iteration is continued until $\underline{\Delta h}$ becomes small and another time step is started. Note that for nonlinear transient problems, the formation and factoring of the system matrix several times during each time step could make the solution process very expensive. One possible way of reducing the cost is to linearize the problem about the initial conditions at t_0 (that is, assume that transmissivities remain fairly constant for all time) and solve Eq. 4.18 directly using $\underline{\underline{M}}_0$ and $\underline{\underline{K}}_0$ at time t_0. Alternatively, if the system matrix is not reformed at every

iteration, some time may be saved. This is effectively the same as linearizing over a couple of iterations. These options are available in AQUIFEM-1.

As a final note, it is important to realize that $\underline{M}_{n+1}^{(i)}$ may change drastically between iterations if the status of the aquifer at a given node is changing between confined and unconfined conditions. This is because the storativity changes by several orders of magnitude during such transitions. The family of time schemes presented here is not designed to accurately handle such strong nonlinearities, so care and engineering judgement may be necessary when modeling these situations.

4.4 Convergence of the Time Integration Scheme

The last question to discuss involves the stability and convergence of the family of methods for time integration of unsteady problems. As in Section 4.3 it is convenient to work with a simple scalar case (Eq. 4.6) and to generalize the results to the groundwater equations.

It is desired to solve Eq. 4.6 as accurately as possible at time t_{n+1} given a solution at time t_n. Thus using the notation h_n, v_n introduced above for the approximate solutions, the following equation is assumed to hold at time t_n:

$$v_n + \lambda h_n = 0 \tag{4.20}$$

Substituting the finite difference expression, Eq. 4.13, gives the result (Eq. 4.15):

$$h_{n+1} = A\, h_n \tag{4.21}$$

where

$$A = \frac{1-(1-\alpha)\Delta t \ \lambda}{1 + \alpha\Delta t\lambda}$$

is known as an *amplification factor*. Note the similarity between Eqs. 4.21 and 4.8. In some sense A should mimic the behavior of $\exp(-\lambda\Delta t)$, hence it is required that

$$|A| < 1 \tag{4.22}$$

This results in the *stability* criteria for the family of methods with parameter α. It can be shown that

for $0 \leq \alpha < \frac{1}{2}$, the stability depends on $\lambda\Delta t$, i.e., the method is *conditionally stable*

for $\frac{1}{2} \leq \alpha \leq 1$, the method is *unconditionally stable.*

In practice therefore it is desirable to choose $\frac{1}{2} \leq \alpha \leq 1$ so that the solution will never "blow up." Figure 4.2 illustrates the way various members of the family approximate $\exp(-\lambda\Delta t)$.

The concept of stability introduced above is quite distinct from that of *convergence*. To discuss convergence a few more definitions are needed. At each time step, the approximate numerical solution of Eq. 4.6 satisfies Eq. 4.21, viz.

$$h_{n+1} - Ah_n = 0 \tag{4.23}$$

However, computing the equivalent of the left-hand side using the exact solutions $h(t_{n+1})$, $h(t_n)$ results in the following expression:

$$h(t_{n+1}) - Ah(t_n) = \tau(t_n) \tag{4.24}$$

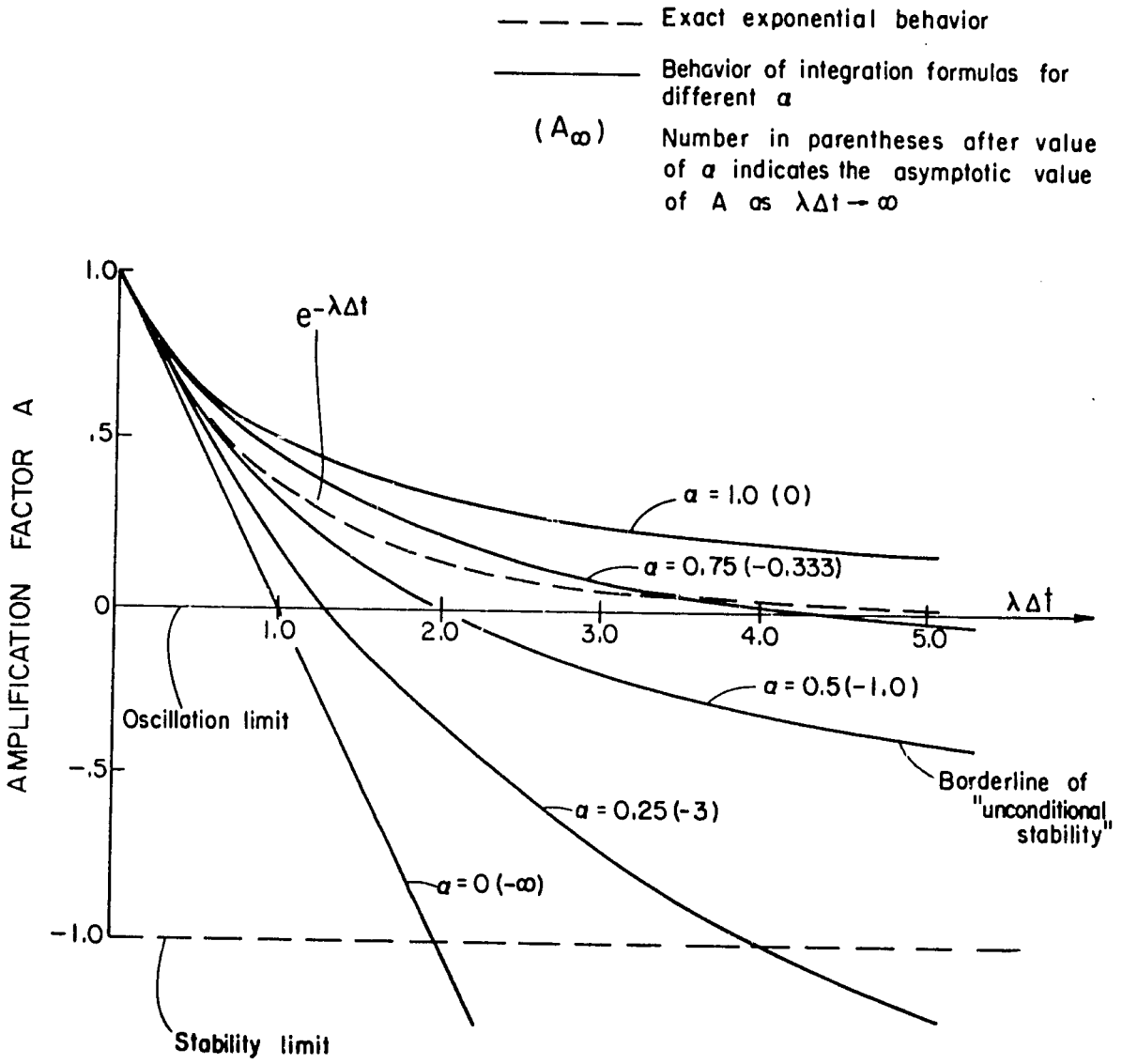

Figure 4.2 Characteristics of Family of Time Integration Methods.

where $\tau(t_n)$ is called the *local truncation error*. An algorithm is said to be *consistent* if

$$|\tau(t_n)| \leq C(\Delta t)^{k+1} \tag{4.25}$$

where C is constant and k is the *order of accuracy* or *rate of convergence*. If an algorithm is stable and consistent it can be shown that the error

$$|e(t_n)| = |h(t_n) - h_n| \leq C^*(\Delta t)^k \tag{4.26}$$

where C^* is another constant and this equation is similar in form to Eq. 3.33. It can be shown that the family of methods used here is 1st-order accurate (k=1), except for $\alpha = \frac{1}{2}$ which is 2nd-order accurate (k=2). This indicates that $\alpha = \frac{1}{2}$ is an important and useful special case.

Just as in Section 4.3, it can also be shown that the results described here for the scalar case apply equally well to the groundwater equations of interest (Eq. 3.12). For $\frac{1}{2} \leq \alpha \leq 1$, the α-family is unconditionally stable and for $\alpha = \frac{1}{2}$ the method is 2nd order accurate. It is not quite clear that this result is true for nonlinear problems (see Hughes, 1977), however, numerical tests and evidence by other workers indicate $\alpha = \frac{1}{2}$ to be a good choice under many situations. There is some evidence that $\alpha = 1$ can give better results for some groundwater applications (Pinder, 1976), thus complete flexibility is allowed in AQUIFEM-1. The user can choose α in the range $0 < \alpha \leq 1$.

Finally note that for the vector-valued case, the equivalent of λ in Eq. 4.6, Figure 4.2 etc., is the largest eigenvalue of the generalized eigenproblem

$$(\underline{\underline{K}} - \lambda_i \underline{\underline{M}})\, \underline{\Psi}_i = 0 \tag{4.27}$$

where λ_i, i=1,...,NEQ, are the eigenvalues of the system and $\underline{\Psi}_i$ are the corresponding eigenvectors. It can be shown (Irons, 1970) that

$$\lambda_{max} \leq \max_{\ell=1,NUMEL} \left(\max_{i=1,3} \lambda_i^e \right) \tag{4.28}$$

where the λ_i^e are solutions of element eigenproblems corresponding to Eq. 4.27. That is, the largest element eigenvalue for all elements is also the largest eigenvalue of the whole system. Unfortunately the largest eigenvalue cannot be obtained analytically for general arbitrarily shaped triangular elements, however λ_{max} can be written in the form

$$\lambda_{max} \leq \max_{\ell=1,NUMEL} \left(\frac{CT}{L^2 S} \right) \tag{4.29}$$

where C is a constant (empirically of the order of 3 or 4) and L, T and S are characteristic values of the element size, transmissivity and storativity, respectively.

The results obtained above are useful for estimating stable time steps, or in the case of unconditionally stable algorithms, for estimating the largest time step that can be expected to give good accuracy. It is certainly preferable to choose $\frac{1}{2} \leq \alpha \leq 1$ since numerical stability

problems will almost certainly be avoided. (Even so, it is remotely possible that for unusual combinations of geometry and boundary conditions, and possibly after many time steps, *roundoff error* in the computer could cause numerical problems.) It remains to decide on an appropriate time step. In order to achieve good accuracy immediately after abrupt changes in boundary conditions, it has been found that irrespective of the value of α, choosing Δt near the stability limit for $\alpha = 0$ is sufficiently small. From Figure 4.2, the stability limit for $\alpha = 0$ is the point at which A reaches -1.0, that is, at $\lambda\Delta t = 2$. From Eq. 4.29, the critical time step for $\alpha = 0$ is thus given by

$$\Delta t_{crit,\alpha=0} = \frac{2}{\lambda_{max}} = 2\left(\frac{L^2S}{CT}\right)_{max} \tag{4.30}$$

A good time step for accuracy with $\frac{1}{2} \leq \alpha \leq 1$ can thus be estimated by evaluating the ratio L^2S/T for the critical elements in the grid (these are obviously the smallest elements, or those with the smallest aquifer storage coefficients or largest transmissivities). The appropriate time step after sudden stresses on the aquifer is then approximately given by:

$$\Delta t \lesssim \left(\frac{L^2S}{T}\right)_{max} \tag{4.31}$$

It is often satisfactory to increase Δt beyond this value at later times and AQUIFEM-1 provides several methods of doing this. Nevertheless Eq. 4.26 shows that the error between exact and numerical solutions is smaller for smaller Δt. Naturally, the initial Δt can be set to a value larger than Eq. 4.31 with a slight loss of accuracy. Solving

the same problem with different size time steps can thus give some indication of the accuracy of the results.

Chapter 5

MODEL VERIFICATION

Several well-known test cases were simulated with AQUIFEM-1 to establish its validity and accuracy for solving groundwater flow problems. In this chapter, comparisons are made with analytical solutions for problems with relatively simple geometry and flow conditions. In particular the aquifers modeled are either one-dimensional (Figure 5.1) or two-dimensional with radial symmetry (Figure 5.2). They are also homogeneous and isotropic with constant bottom elevation and thickness. Both steady and transient cases are treated.

5.1 One-Dimensional Steady State Problems

A series of very simple one-dimensional steady state tests are examined first.

Test Case 1: Confined aquifer with prescribed head boundary conditions.

The partial differential equation (PDE) for one dimensional steady flow in a homogeneous confined aquifer is:

$$\text{PDE:} \quad \frac{\partial}{\partial x}\left(T_{xx}\frac{\partial \phi}{\partial x}\right) = 0 \quad \text{or} \quad \frac{d^2\phi}{dx^2} = 0 \tag{5.1}$$

since $T_{xx} = K_{xx}B$ is independent of both x and ϕ. For this test, the boundary conditions (BC) are:

$$\text{BC:} \quad \begin{aligned} \phi &= \phi_0 \text{ at } x = 0 \\ \phi &= \phi_L \text{ at } x = L \end{aligned} \tag{5.2}$$

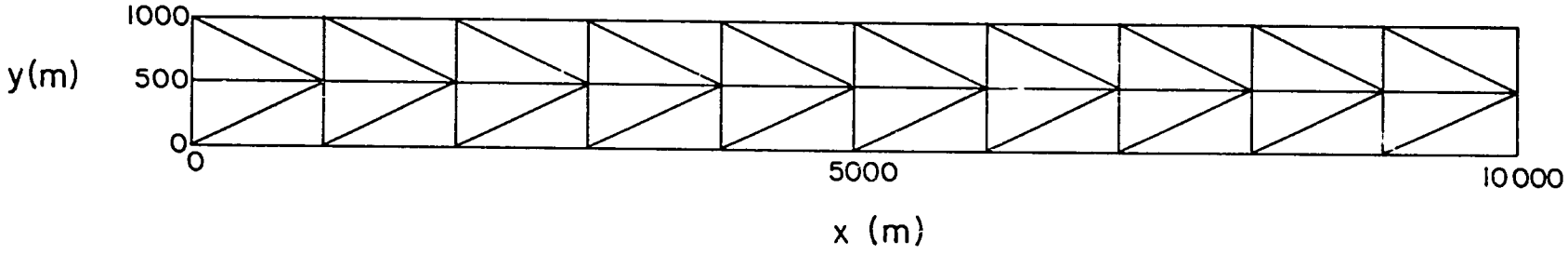

Figure 5.1 Finite Element Grid for One Dimensional Problems.

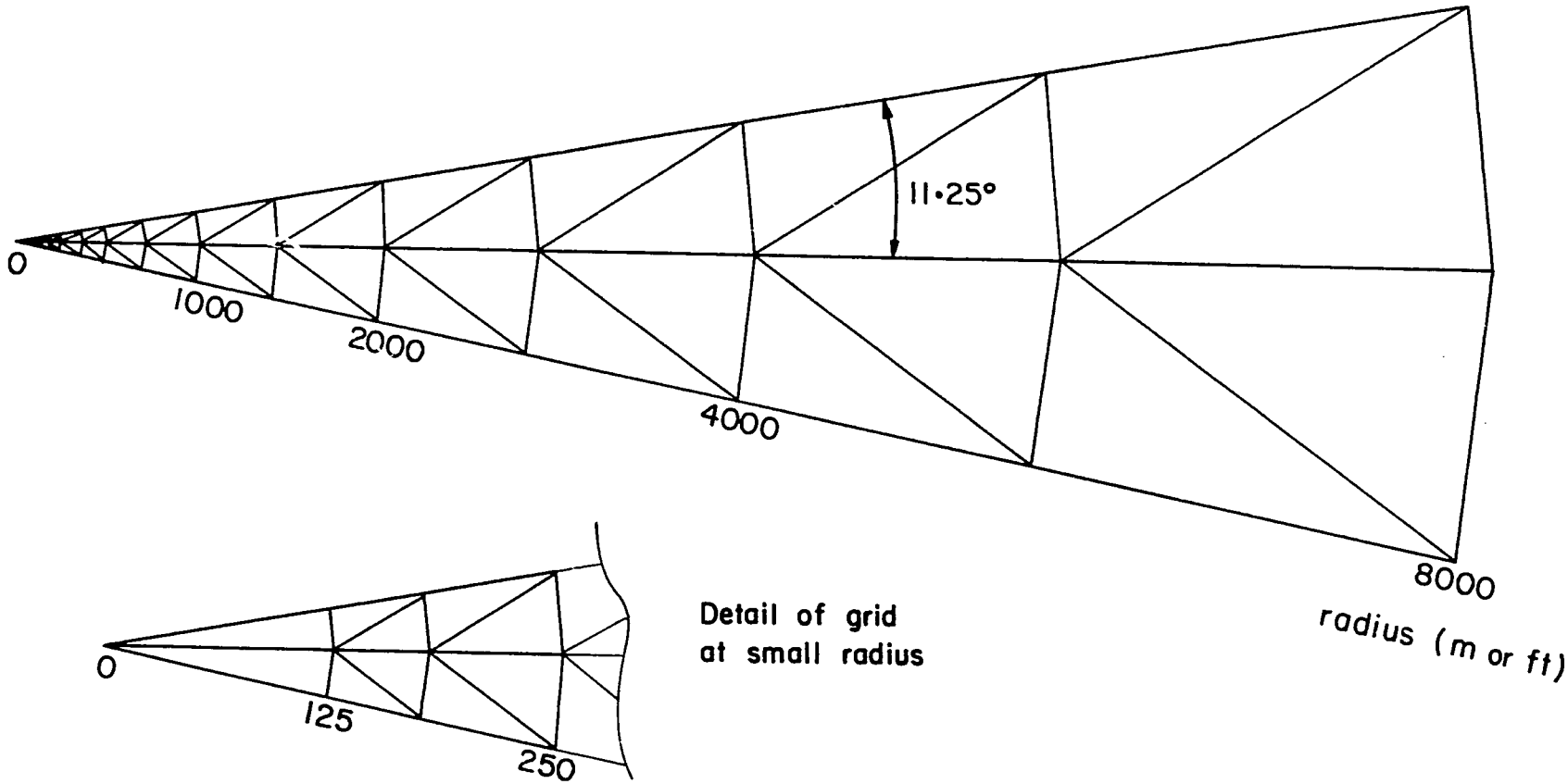

Figure 5.2 Finite Element Grid for Radially Symmetric Problems.

and the solution is obtained by direct integration:

$$\phi = \phi_o + \frac{\phi_L - \phi_o}{L} x \tag{5.3}$$

Note that the solution is independent of the transmissivity, however the flux per unit width of aquifer, $Q_x [L^2/T]$, is given by

$$Q_x = -T_{xx} \frac{\partial \phi}{\partial x}$$

$$= T_{xx} \frac{(\phi_o - \phi_L)}{L} \tag{5.4}$$

which depends directly on transmissivity.

The following parameters are used in the numerical test:

Bottom elevation	$z = 0$ m
Thickness	$B = 20$ m
Transmissivity	$T_{xx} = 20000$ m^2/day
Aquifer length	$L = 10000$ m
Prescribed heads	$\phi_o = 100$ m
	$\phi_L = 50$ m

Substituting these values in Eqs. 5.3 and 5.4 gives the exact solutions,

$$\phi = 100 - 0.005\ x \quad (m) \tag{5.5}$$

and

$$Q_x = 100\ (m^2/day)\ . \tag{5.6}$$

The results from AQUIFEM-1 depend on the computer and word-length

employed. Thus, double precision on an IBM 370 gives the exact solution for ϕ and Q_x to at least five significant figures, whereas single precision results show minor round-off error. Figure 5.3 illustrates the exact and numerical solutions.

Test Case 2: Phreatic aquifer with prescribed head boundary conditions.

$$\text{PDE:} \quad \frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right) = K_{xx}\frac{d}{dx}\left(h\frac{dh}{dx}\right) = 0 \tag{5.7}$$

where for a phreatic aquifer with zero bottom elevation, $T_{xx} = K_{xx}h$ depends on the water surface elevation, however, K_{xx} is independent of x since the aquifer is homogeneous.

$$\text{BC:} \quad \begin{aligned} h &= h_o \quad \text{at } x = 0 \\ h &= h_L \quad \text{at } x = L \end{aligned} \tag{5.8}$$

Solution (by integration):

$$h^2 = h_o^2 + \frac{h_L^2 - h_o^2}{L}\, x \tag{5.9}$$

$$\begin{aligned} Q_x &= -K_{xx}h\frac{\partial h}{\partial x} \\ &= K_{xx}\frac{(h_o^2 - h_L^2)}{2L} \end{aligned} \tag{5.10}$$

The parameters for the numerical test are:

Bottom elevation	z = 0 m
Thickness	B = 120 m

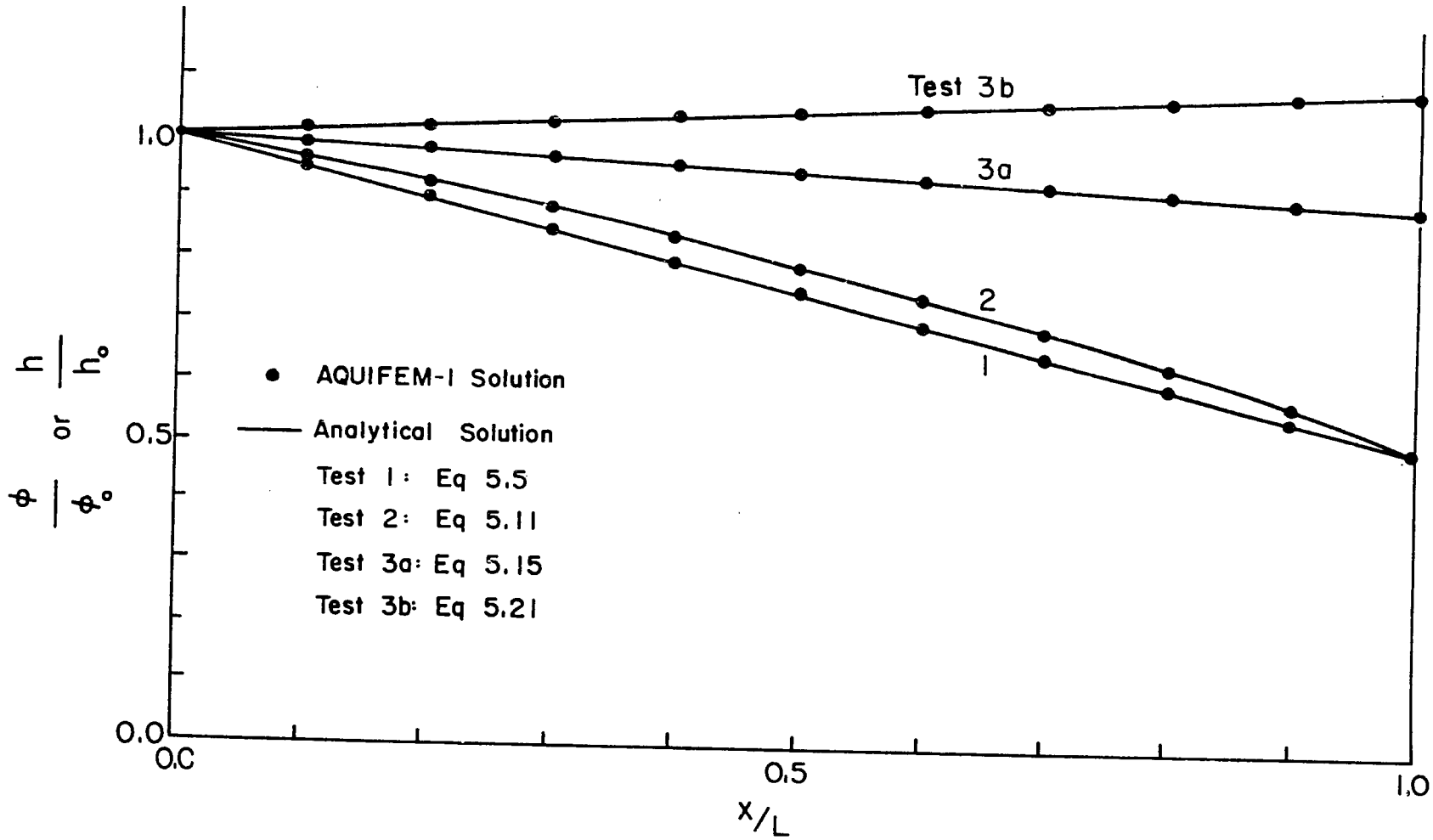

Figure 5.3 One-Dimensional Steady State Tests.

Permeability	K_{xx} = 1000 m/day
Aquifer length	L = 10000 m
Prescribed heads	h_o = 100 m
	h_L = 50 m

Hence the exact solution becomes

$$h^2 = 10000 - 0.75\ x\ (m^2) \tag{5.11}$$

and

$$Q_x = 375\ (m^2/day)\ . \tag{5.12}$$

Now unlike Eq. 5.1, Eq. 5.7 is nonlinear in the unknown h. This means that the numerical results depend not only on round-off error, but also on the iteration scheme used, the initial guess and the convergence criterion. For this steady state problem, AQUIFEM-1 uses fixed-point iteration as given in Eq. 4.3. The piezometric heads shown in Figure 5.3 are computed with the left-hand side matrix $\underline{K}^{(i)}$ being updated every two iterations (NSYS=2). The method seems to converge well for a wide range of initial guesses. Thus, for example, the results shown are computed with a linear initial guess which is comptuted by a useful program option in AQUIFEM-1. Three iterations are required in this case until the root mean square error (Eq. 4.4, ITOL=0) is less than 0.05 (TOL). For this test case, the computed flux Q_x varies in the range 366.985 to 377.804 m^2/day at different nodes, these worst results being near x = L where $\partial h/\partial x$ is greatest. Some inaccuracy in fluxes is to be expected, however, when linear triangular elements are used.

Test Case 3: Confined aquifer with leaky inflows.

(a) Leakage from an adjacent aquifer.

$$\text{PDE:} \quad T_{xx} \frac{d^2\phi}{dx^2} + \frac{K'}{B'} (\phi_a - \phi) = 0 \tag{5.13}$$

where T_{xx} = KB, K'/B' and ϕ_a are all constant.

$$\text{BC:} \quad \begin{aligned} \phi &= \phi_o \quad \text{at } x = 0 \\ \phi &= \phi_L \quad \text{at } x = L \end{aligned} \tag{5.14}$$

Solution (by standard methods of solving linear differential equations):

$$\phi = \phi_a + (\phi_o - \phi_a) \frac{\sinh[a(L-x)]}{\sinh(aL)} + (\phi_L - \phi_a) \frac{\sinh(ax)}{\sinh(aL)} \tag{5.15}$$

where:

$$a = \sqrt{\frac{K'}{B' K_{xx} B}}$$

and

$$Q_x = -T_{xx} \frac{\partial\phi}{\partial x}$$

$$= aT_{xx} \left[(\phi_o - \phi_a) \frac{\cosh[a(L-x)]}{\sinh(aL)} - (\phi_L - \phi_a) \frac{\cosh(ax)}{\sinh(aL)} \right] \tag{5.16}$$

To test this case numerically, the following parameters are used:

Bottom elevation	z = 0
Thickness	B = 20 m
Transmissivity	T_{xx} = 20000 m^2/day

Aquifer length	$L = 10000$ m
Leaky layer parameter	$K'/B' = 0.0002\ \text{day}^{-1}$
Head in adjacent aquifer	$\phi_a = 95$ m
Prescribed heads	$\phi_o = 100$ m
	$\phi_L = 90$ m

A comparison between the analytical and computed heads is shown in Table 5.1 and Figure 5.3. In double precision, the computed heads are correct to at least five significant figures. As in Test Case 2, however, there is some error in the computed fluxes (which are shown in Table 5.1, averaged over three nodes at the same x location).

(b) <u>Leakage at a 3rd-type boundary at one end of domain.</u>

$$\text{PDE:}\quad \frac{\partial}{\partial x}\left(T_{xx}\frac{\partial\phi}{\partial x}\right) = 0 \rightarrow \frac{d^2\phi}{dx^2} = 0 \tag{5.17}$$

where $T_{xx} = K_{xx}B$ is constant.

$$\text{BC:}\quad \phi = \phi_o \text{ at } x = 0 \quad \text{(1st-type)}$$

$$-T_{xx}\frac{\partial\phi}{\partial x} = \frac{K''W''}{B''}(\phi-\phi_3) \quad \text{at } x = L \quad \text{(3rd-type)} \tag{5.18}$$

Solution (by integration):

$$\phi = \phi_o + \frac{\phi_3-\phi_o}{\left(\frac{B''K_{xx}B}{K''W''} + L\right)}x \tag{5.19}$$

Table 5.1 Solutions to Test Case 3a

Location	Piezometric head		Flux per unit width	
	ϕ(m)		$Q = -T_{xx} \frac{\partial \phi}{\partial x}$ [m^2/day]*	
	Analytical (Eq. 5.15)	AQUIFEM-1	Analytical (Eq. 5.16)	AQUIFEM-1**
0	100.000	100.000	21.640	21.174
1000	98.941	98.941	20.746	20.736
2000	97.922	97.922	20.060	20.061
3000	96.932	96.932	19.575	19.587
4000	95.961	95.961	19.286	19.308
5000	95.000	95.000	19.190	19.223
6000	94.039	94.039	19.286	19.330
7000	93.068	93.068	19.575	19.630
8000	92.078	92.078	20.060	20.126
9000	91.059	91.059	20.746	20.824
10000	90.000	90.000	21.640	21.174

Notes: *T_{xx} and all other parameters and boundary conditions are described in the text.

**Average of three values at same x location.

and

$$Q_x = \frac{K_{xx}B(\phi_o - \phi_3)}{\left(\frac{B''K_{xx}B}{K''W''} + L\right)} \tag{5.20}$$

Note the similarity between this solution and Eqs. 5.3 and 5.4. The effect of the 3rd-type boundary is the same as if the aquifer were stretched to an effective length which is longer than L by the amount (B"KB)/(K"W").

In the numerical test, the following parameters are used:

Bottom elevation	$z = 0$ m
Thickness	$B = 20$ m
Transmissivity	$T_{xx} = 20000$ m/day
Aquifer length	$L = 10000$ m
Prescribed head	$\phi_o = 100$ m
Head at 3rd-type boundary	$\phi_3 = 120$ m
3rd-type boundary parameter	$K''W''/B'' = 2$ m/day

The exact solutions are thus

$$\phi = 100 + 0.001\ x \quad (m) \tag{5.21}$$

and

$$Q_x = -20\ (m^2/day)\ . \tag{5.22}$$

The numerical solution for ϕ (shown in Figure 5.3) and Q_x is correct to at least five significant figures when computed in double precision.

5.2 Unsteady Problems

In this section, numerical solutions to groundwater problems are compared with a number of analytical solutions in both one-dimensional and radially symmetric situations. In two cases, only approximate analytical solutions are available.

Test Case 4: One-dimensional confined aquifer

PDE: $$S \frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x} \left(T_{xx} \frac{\partial \phi}{\partial x}\right) = T_{xx} \frac{\partial^2 \phi}{\partial x^2} \tag{5.23}$$

where T_{xx} is constant.

BC: $$\begin{aligned} \phi &= \phi_o \quad \text{at } x = 0,\ t > 0 \\ \phi &= \phi_o/2 \quad \text{at } x = L,\ t > 0 \end{aligned} \tag{5.24}$$

Initial condition (IC):

IC: $$\phi = \phi_o \quad \text{at } t = 0,\ 0 \leq x \leq L \tag{5.25}$$

Solution (see for example Carslaw and Jaegar, 1959, Section 3.4):

$$\phi = \phi_o - \frac{\phi_o}{2} \frac{x}{L} + \frac{\phi_o}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} \exp\left(- \frac{T_{xx} n^2 \pi^2 t}{SL^2}\right) \sin\left(\frac{n\pi x}{L}\right) \tag{5.26}$$

This result is plotted in Figure 5.4 at several times, together with AQUIFEM-1 numerical solutions computed with the grid shown in Figure 5.1 and the following parameters:

Bottom elevation	z = 0 m
Thickness	B = 20 m

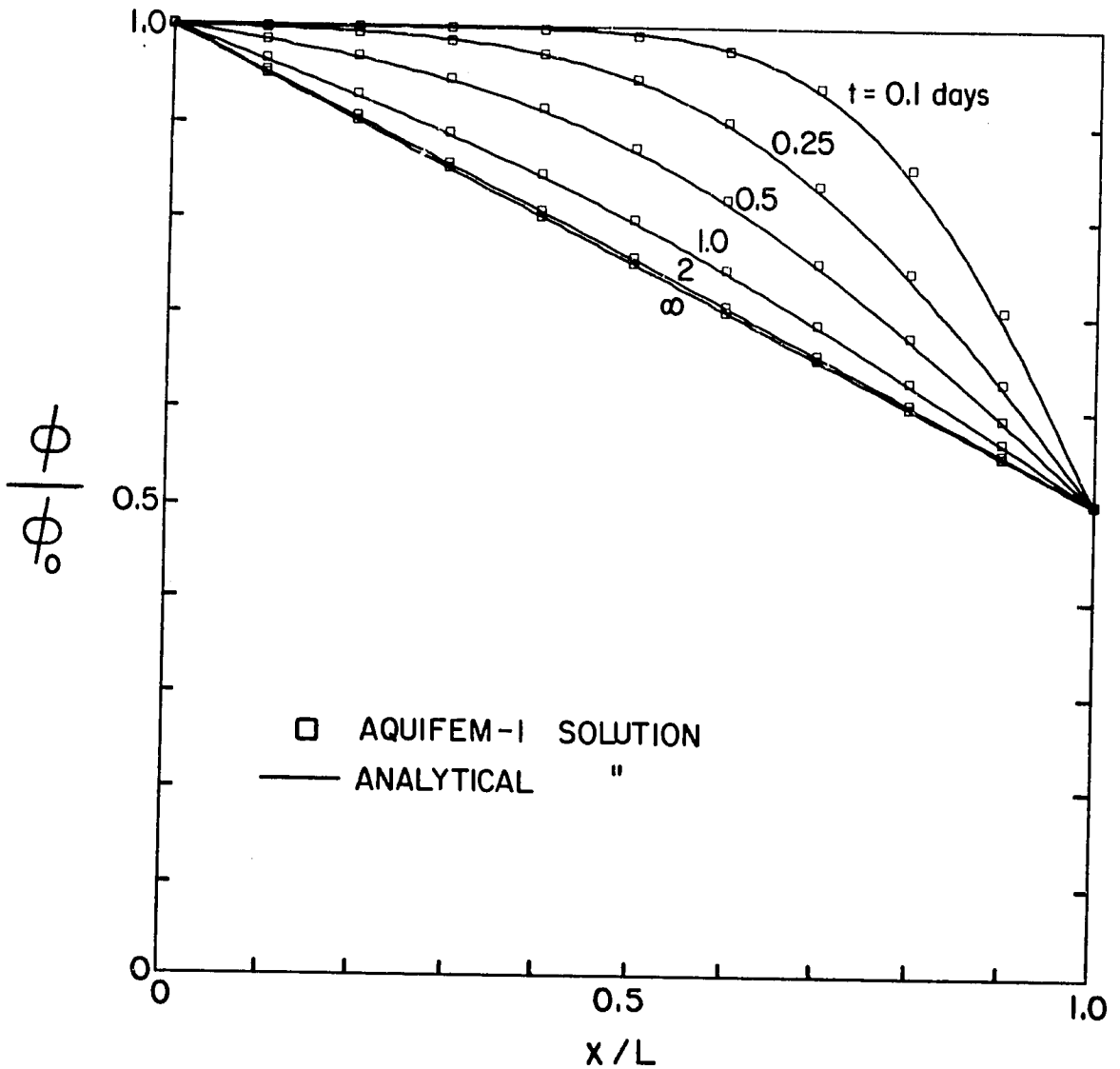

Figure 5.4 One Dimensional Transient Test.

Transmissivity	$T_{xx} = 20000\ m^2/day$
Storativity	$S = 0.001$
Aquifer length	$L = 10000\ m$
Initial piezometric head	$\phi_0 = 100\ m$
Initial time step	$\Delta t = 0.02$ days
Multiplicative factor for increasing successive time steps*	DTPARM = 1.2
Special solution times, requiring modification of time steps*	0.1, 0.25, 0.5, 1.0, 2.0, 3.0 days
Time integration parameter	$\alpha = 0.7$

Note that the initial time step is 0.4 times the value of the quantity

$$\frac{(\Delta x)^2 S}{T_{xx}} \sim \frac{(1000)^2 \times 0.001}{20000} = 0.05 \text{ days},$$

and Section 4.4 suggests that this time step should give good accuracy. Indeed Figure 5.4 shows good agreement, and the numerical solution approaches the final steady state solution at large times. Solutions computed with $\alpha = 0.5$ and $\alpha = 1.0$ do not differ greatly from the solution shown here. Although the former underestimates the drawdown at early times and the latter underestimates at large times, these differences would not be serious in a real-world application.

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*Note: These program features are described by Townley and Wilson, 1980.

Test Case 5: Confined aquifer - radial flow to a well with no leakage

PDE: $$S \frac{\partial \phi}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (r\, T_{rr} \frac{\partial \phi}{\partial r}) \quad , \quad 0 \leq r$$

or $$S \frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x} (T_{xx} \frac{\partial \phi}{\partial x}) + \frac{\partial}{\partial y} (T_{yy} \frac{\partial \phi}{\partial y})$$

$$= T \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) \quad \text{for all } x,y \tag{5.27}$$

where $T = T_{rr} = T_{xx} = T_{yy}$ is constant.

BC: $$\phi = \phi_0 \quad \text{as } r \to \infty, \quad t > 0$$

$$\lim_{r \to 0} r \frac{\partial \phi}{\partial r} = \frac{Q}{2\pi T} \quad \text{as } r \to 0, \quad t > 0 \tag{5.28}$$

IC: $$\phi = \phi_0 \quad \text{at } t = 0,\ r \geq 0 \tag{5.29}$$

Solution (see for example Bear, 1979, but originally due to Theis):

$$\phi = \phi_0 - \frac{Q}{4\pi T} W(u) \tag{5.30}$$

where

$$u = \frac{r^2 S}{4Tt}$$

and the Theis *Well Function* W(u) is given by

$$W(u) = \int_u^\infty \frac{e^{-z}}{z} dz$$

and is tabulated in various groundwater references (e.g., Hantush, 1964; Bear, 1979).

Since it is not possible to numerically model an infinite aquifer with radial flow towards a well, the grid shown in Figure 5.2 is truncated at a finite radius from the well. This means that the boundary condition at infinity (Eq. 5.28) is approximated in the numerical model by applying it at the nodes farthest from the well, and the well boundary condition is applied at a single node. Because of radial symmetry only a 22.5^{o} slice of the aquifer is modeled and the total flux pumped at the well node is only 1/16th of Q in the above equations.

In the numerical test of this problem the following parameters are used:

Bottom elevation	$z = 0$ m
Thickness	$B = 100$ m
Transmissivity	$T = 100{,}000\ m^2/day$
Storativity	$S = 0.001$
Initial piezometric head	$\phi_o = 100$ m
Well pumping rate	$Q = 160{,}000\ m^3/day$
Initial time step	$\Delta t = 0.00003$ days
Multiplicative factor for increasing successive time steps	DTPARM = 1.25
Time integration parameter	$\alpha = 0.7$

Figure 5.5 compares the analytical Theis curve with the numerical

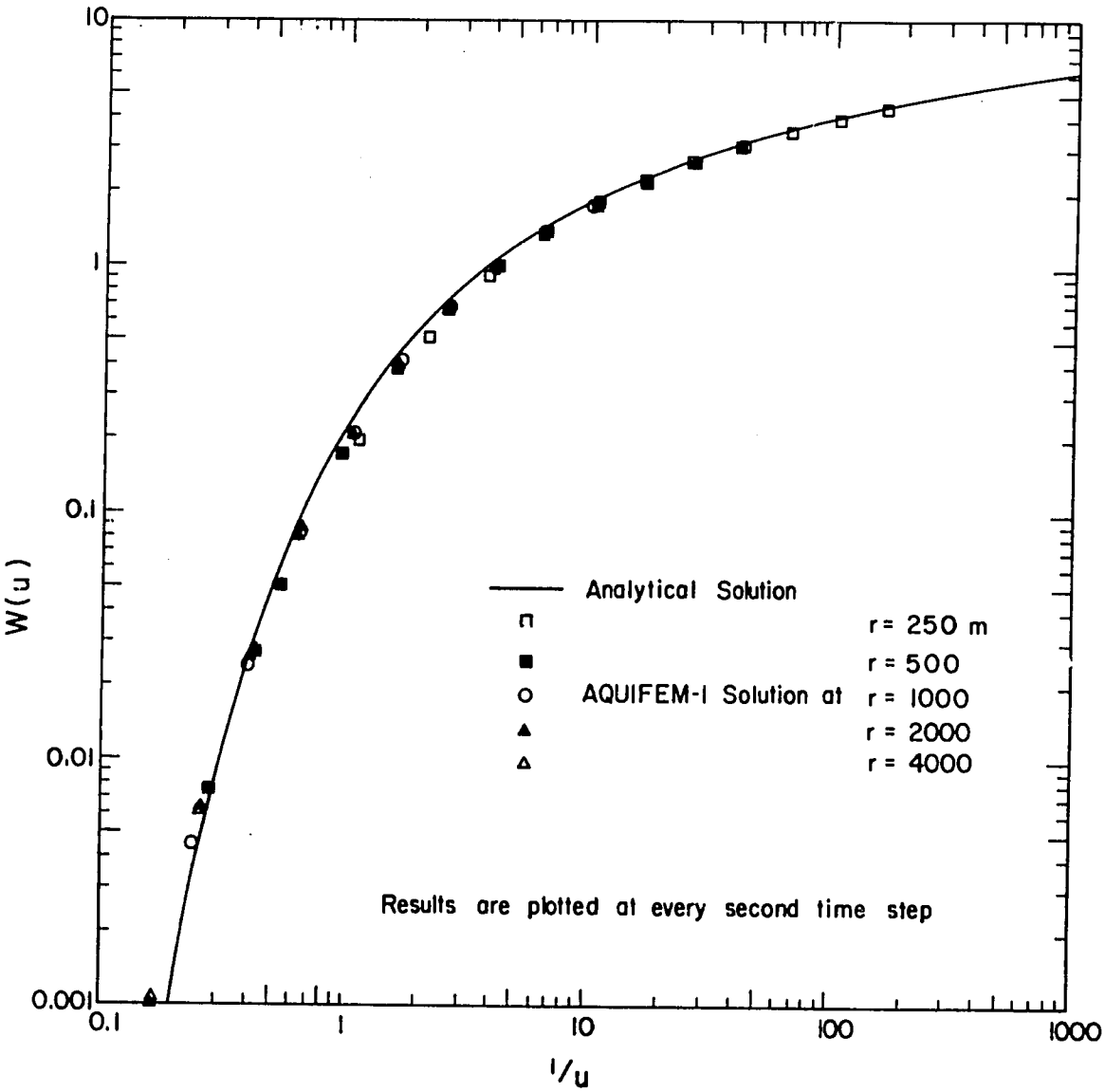

Figure 5.5 Numerical Simulation of Theis Curve.

solution. Agreement is reasonably good; however, at small times, corresponding to small 1/u, the numerical solution varies with different values of α. Specifically, the predicted drawdown increases as α increases for 1/u less than one.

In this test case, the parameter

$$\frac{(\Delta x^2)S}{T} \sim \frac{(51.8)^2 \times 0.001}{10000} = 0.000027 \text{ days}$$

which is very close to the initial time steps. (The critical value of Δx used here is the length in the radial direction of the smallest elements near the well.) At large times, the time step is much greater than this value; however, this causes no problem since the time integration scheme is unconditionally stable. Note that there is no final steady state solution for this problem.

<u>Test Case 6</u>: <u>Confined aquifer - radial flow to a well with leakage</u>

$$\text{PDE:} \quad S\frac{\partial\phi}{\partial t} = T\left(\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2}\right) + \frac{K'}{B'}(\phi-\phi_a) \tag{5.31}$$

which is modified in the same way as Eq. 5.27, and where K'/B' (leaky layer properties) and ϕ_a (the head in the adjacent aquifer) are constant. It is assumed here that the leakage derived from storage in the semipervious layer is negligible.

BC: See Eq. 5.28

IC: See Eq. 5.29

Solution (see for example, Hantush, 1964, and Bear, 1979, but originally due to Hantush and Jacob) for the special case where $\phi_a \equiv \phi_o$:

$$\phi = \phi_o - \frac{Q}{4\pi T} W(u, r/\beta) \tag{5.32}$$

where again

$$u = \frac{r^2 S}{4Tt}$$

and

$$\beta = \sqrt{\frac{T}{K'/B'}}$$

is the inverse of the parameter "a" appearing in Eq. 5.15. The *leaky well function* $W(u,r/\beta)$ is given by

$$W(u,r/\beta) = \int_u^\infty \frac{1}{z} \exp(-z - \frac{r^2}{4\beta^2 z}) dz$$

and is also tabulated by Hantush (1964).

A numerical solution to this problem is obtained using the same grid and parameters as in Test Case 5, with the addition of:

Adjacent head	$\phi_a \equiv \phi_o$ = 100 m (as required)
Leaky layer parameters	K'/B' = 0.1 days^{-1}

Figure 5.6 shows the numerical and analytical results for five different distances from the well. Just as in Test Case 5, there are minor discrepancies, particularly near 1/u of the order of one. These errors are not believed to be serious, however, and could be reduced by refining the finite element grid and/or reducing time steps.

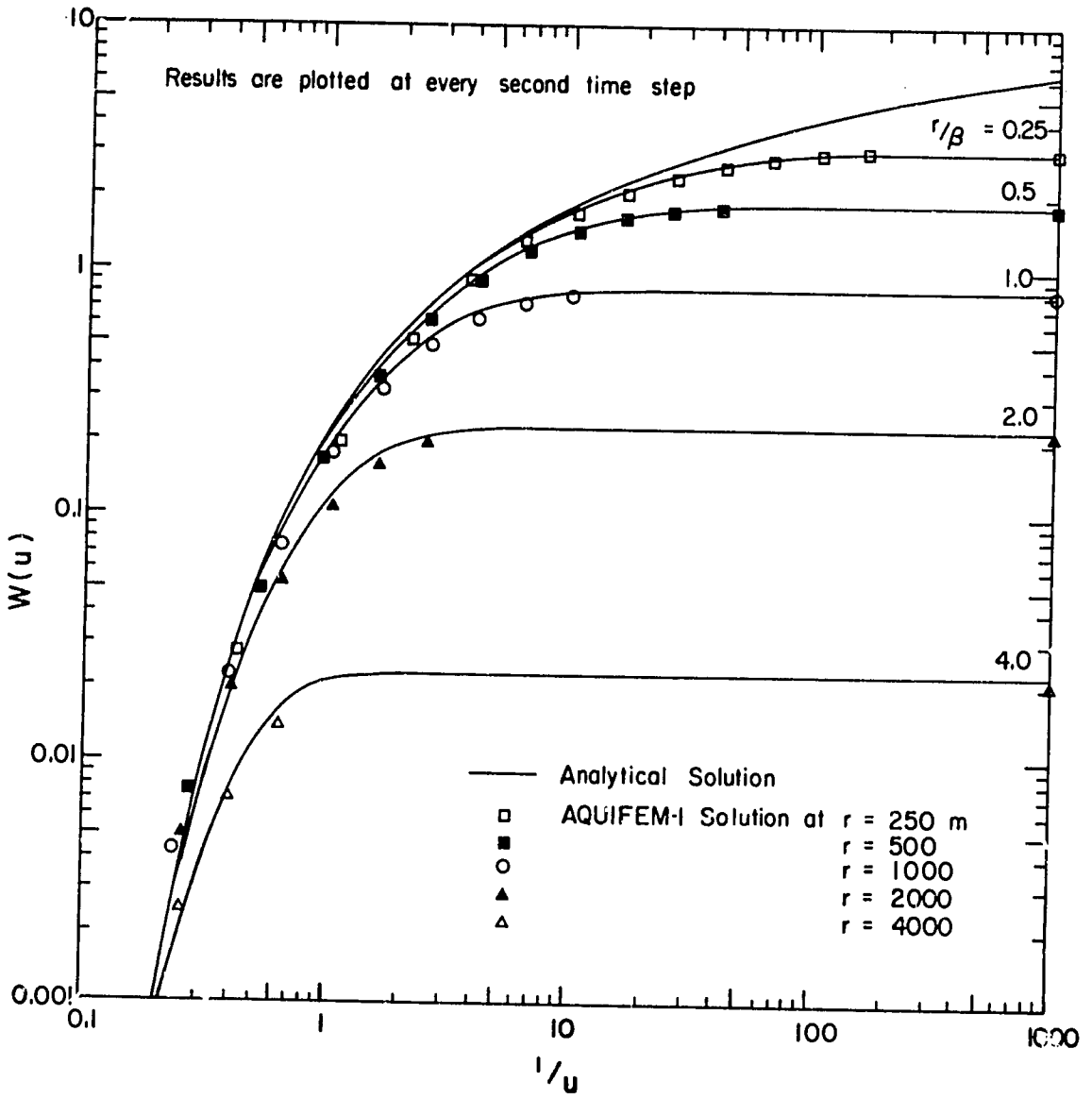

Figure 5.6 Numerical Simulation of Hantush Curves.

The numerical steady state solution underestimates the drawdown at large radii because of the constraining effect of the approximate boundary condition at r = 8000 m and also because of the lumped representation of leakage in AQUIFEM-1. The results suggest that adjacent elements should not vary too greatly in size when leakage is occurring.

Test Case 7: Unconfined one-dimensional aquifer - similarity solution

There are very few analytical solutions for the time-varying location of the phreatic surface in an unconfined aquifer. Indeed the available solutions are either exact solutions of gross physical approximations, or approximate solutions of more realistic physical representations. The analytical solution presented here falls in the former category because the saturated thickness at the boundaries is zero for t > 0.

$$\text{PDE:} \quad S_y \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(T_{xx} \frac{\partial h}{\partial x}\right) = K_{xx} \frac{\partial}{\partial x}\left(h \frac{\partial h}{\partial x}\right) \tag{5.33}$$

where $T_{xx} = K_{xx}h$ and $K_{xx} = K$ is constant.

$$\text{BC:} \quad h = 0 \quad \text{at } x = 0,L;\ t > 0 \tag{5.34}$$

$$\text{IC:} \quad h/h_o = X(x/L);t = 0 \tag{5.35}$$

where $X(x/L)$ is given by:

$$\int_0^X \frac{X dX}{\sqrt{1-X^3}} = 1.72474\left(\frac{x}{L}\right)$$

and is presented in Table 5.2.

Table 5.2 Similarity Profile for Test Case 7

x/L	$\mathbb{X}$
0	0
0.05	0.412
0.10	0.575
0.15	0.692
0.20	0.782
0.25	0.853
0.30	0.908
0.35	0.949
0.40	0.978
0.45	0.994
0.50	1.000

The solution to this problem (see for example, Bear, Zaslavsky and Irmay, 1969, or Glover, 1974, but originally due to Boussinesq) is based on the hypothesis that a *similarity* solution exists which maintains its fundamental shape in time. Given this hypothesis, a critical part of the solution procedure is the determination of the appropriate initial conditions so that this can occur. The solution is:

$$h/h_o = \frac{\mathbb{X}(x/L)}{4.46209\left(\frac{Kh_o t}{S_y L^2}\right) + 1} \tag{5.36}$$

Numerically the following parameters are used to simulate this situation:

Bottom elevation	$z = 0$ m
Thickness	$B = 110$ m
Hydraulic conductivity	$K = 10000$ m/day
Specific yield	$S_y = 0.1$
Aquifer length	$L = 20000$ m
Initial head at $x = L/2$	$h_o = 100$ m
Initial time step	$\Delta t = 0.05$ days
Multiplicative factor for increasing successive time steps	DTPARM = 1.2
Special solution times, requiring modification of time steps	2.988, 8.964, 26.89 days
Time integration parameter	$\alpha = 0.5$
Maximum number of iterations*	MAXIT = 5
Tolerance for convergence* (root mean square error criterion)	TOL = 0.01
Number of iterations between rebuilding system matrix*	NSYS = 1

Because of the axis of symmetry at $x = L/2$, only half of the aquifer is modeled with AQUIFEM-1, that is $0 \leq x \leq L/2$. Figure 5.7 compares the analytical and numerical solutions. It can be seen that

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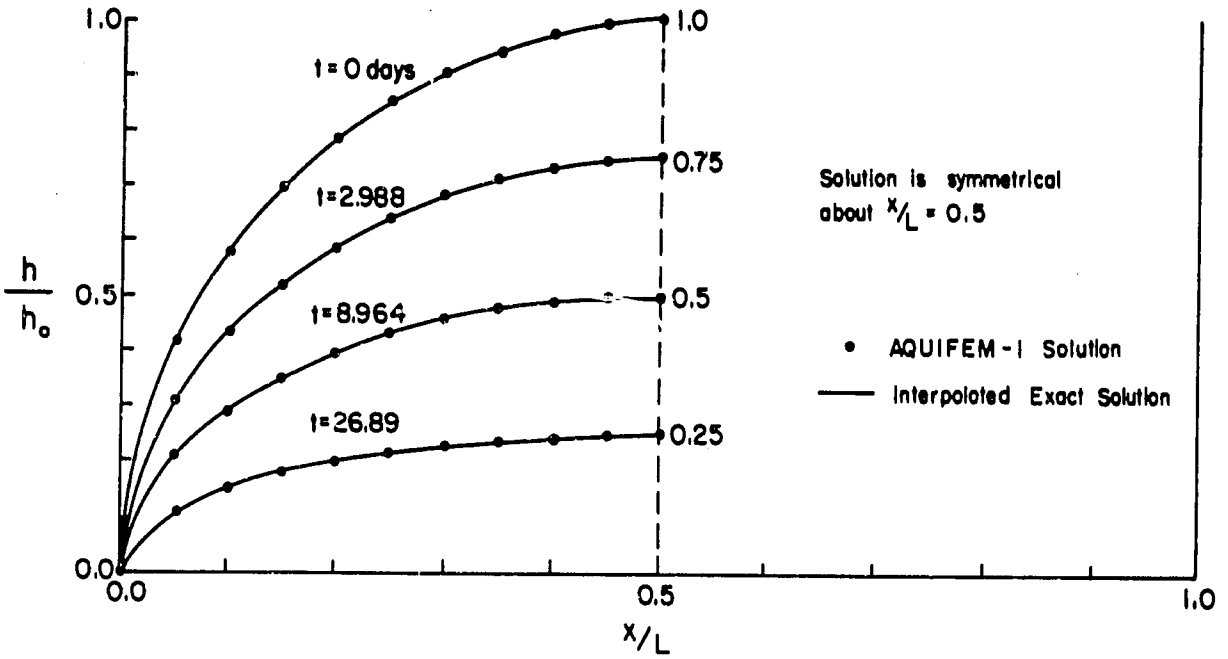
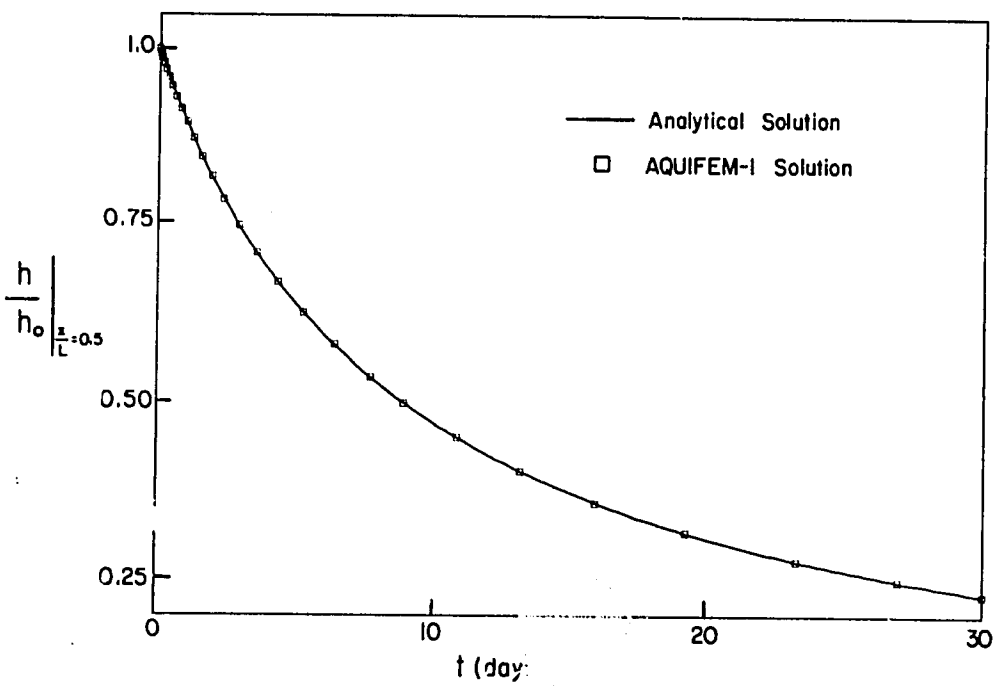
*Note: These program parameters are described by Townley and Wilson, 1980.



a) Decay of Groundwater Mound with Time



b) Variation of Head at Center of Aquifer with Time

Figure 5.7 Similarity Solution for Groundwater Mound.

AQUIFEM-1 performs remarkably well, all piezometric heads being correct to at least three significant figures.

Test Case 8: Radial flow to a well with change of status

Test Case 5 considered the case of a pumping well in a confined aquifer where the initial head ϕ_0 was much greater than the top elevation of the aquifer, (z + B). If ϕ_0 is only slightly greater than (z + B), however, then as pumping continues, the head near the well can drop below the top of the aquifer and the aquifer converts locally from confined to water table conditions. This is a difficult situation to handle numerically since the aquifer storage coefficient is usually orders of magnitude different on either side of the line of transition. In this test problem, this situation is simulated using AQUIFEM-1.

Let the radius at which transition occurs be R. There are then different PDE's which apply in the different regions of the aquifer:

$$\text{PDE's:} \quad S_y \frac{\partial h}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\, T_{rr} \frac{\partial h}{\partial r}\right), \quad 0 \le r \le R$$

$$S \frac{\partial \phi}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\, T_{rr} \frac{\partial \phi}{\partial r}\right), \quad r \ge R \tag{5.37}$$

$$\text{where} \quad T_{rr} = \begin{cases} K_{rr}h & \text{in the phreatic region} \\ K_{rr}B & \text{in the confined region,} \end{cases}$$

K_{rr} = K is assumed to be constant and there are *matching conditions* at the radius of transition R:

$$h = \phi = B \quad \text{at } r = R,\ t > 0$$

$$\frac{\partial h}{\partial r} = \frac{\partial \phi}{\partial r} \quad \text{at } r = R,\ t > 0 \tag{5.38}$$

BC:

$$\phi = \phi_o \quad \text{as } r \to \infty,\ t > 0$$

$$\lim_{r \to 0} rh \frac{\partial h}{\partial r} = \frac{Q}{2\pi K} \quad \text{as } r \to 0,\ t > 0 \tag{5.39}$$

IC: $\phi = \phi_o$ at $t = 0$, $r \geq 0$ (5.40)

There is no exact solution for the problem defined here, however, if the drawdown below the top of the aquifer in the phreatic region is small compared to the aquifer thickness (that is, $(B-h)/B << 1$), then the PDE in the phreatic can be linearized about $h = B$ and Eqs. 5.37 become

$$S_y \frac{\partial h}{\partial t} = \frac{T}{r} \frac{\partial}{\partial r} \left(r \frac{\partial h}{\partial r}\right), \quad 0 \leq r \leq R$$

$$S \frac{\partial \phi}{\partial t} = \frac{T}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r}\right), \quad r \geq R\ . \tag{5.41}$$

where $T = KB$ is constant. The solution to these approximate equations was first presented in the groundwater literature by Moench and Prickett (1972):

$$h = B - \frac{Q}{4\pi T} [W(u_1) - W(v_1)],\ r < R$$

$$\phi = \phi_o - \frac{Q}{4\pi T} W(u_2) \exp(v_2 - v_1)\ ,\ r \geq R \tag{5.42}$$

where $u_1 = r^2 S_y/4Tt$

$u_2 = r^2 S/4Tt$

$v_1 = R^2 S_y/4Tt$

$v_2 = R^2 S/4Tt = v_1 S/S_y$

W(u) is the well function defined earlier and

v_1 is the root of

$$\frac{Q}{4\pi T} e^{-v_1} = \frac{(\phi_o - B)\, e^{-v_2}}{W(v_2)}$$

These results are presented graphically for different combinations of parameters in their paper.

In order to check the ability of AQUIFEM-1 to simulate problems of this type, an attempt was made to reproduce the results presented in Figures 2 and 3 of Moench and Prickett (1972). In particular, the following parameters were used in a numerical test using the finite element grid shown in Figure 5.2:

Aquifer bottom elevation	$z = 0$ ft
Aquifer thickness	$B = 100$ ft
Transmissivity	$T = 2674.0$ ft^2/day
	$= 20{,}000$ U.S. gpd/ft
Aquifer storativity	$S = 0.0001$
Specific yield	$S_y = 0.1$

Initial piezometric head	ϕ_0 = 102 ft
Well pumping rate	Q = 33636 ft^3/day
	= 251,600 U.S. gpd
Initial time step	Δt = 0.0002 days
Multiplicative factor for increasing successive time steps	DTPARM = 1.1
Tolerance for convergence (absolute deviation criterion)	TOL = 0.05
Time integration parameter	α = 1.0

Figure 5.8a compares the approximate analytical and numerical results at a radius from the well of 1000 ft. The change of drawdown with time is also shown in Figure 5.8b at five different radii, together with the corresponding times of transition from confined to unconfined behavior. In general the time of transition at radius R is given by

$$t = \frac{R^2 S_y}{4Tv_1} \quad , \tag{5.43}$$

where v_1 is defined above. For the parameters used in this test, however, v_1 has the value 1.134 and the times of transition are given by

$$t = 8.24 \times 10^{-6} R^2 \text{ days.}$$

It can be seen that the numerical solution shows the right trends but does not completely reproduce the analytical result. At radii up to 1000 ft, the time of transition is well within engineering accuracy, however at 2000 ft the error is 100 percent. This can be explained

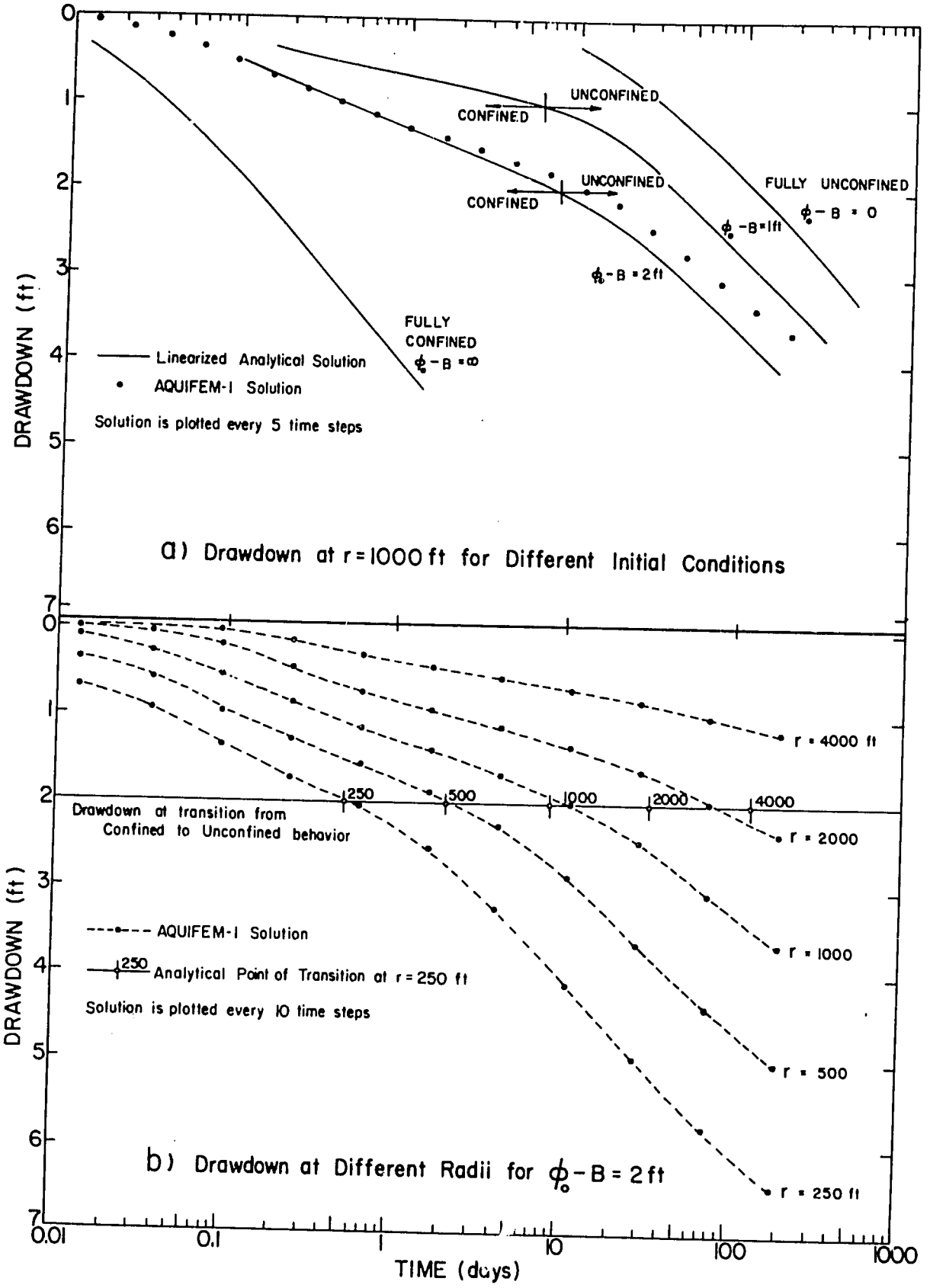


Figure 5.8 Conversion from Confined to Unconfined Behavior.

by considering the effect of the truncated finite element grid and the approximate boundary condition used at r = 8000 ft.

It can be shown from Eq. 5.42 that at a radius r > R, the total flux towards the well is given by

$$2\pi rT \frac{\partial\phi}{\partial r} = Q \exp(v_2 - v_1 - u_2) \tag{5.44}$$

Now the numerical solution for this flux at r = 8000 ft is always in error since the drawdown is constrained to be zero at that radius. However, the error in flux becomes more serious as time increases. At $t \sim 1$ day, the error is about 0.1 Q, and at t = 10 days the error is almost 0.2 Q. Because the drawdown is forced to be zero, the well's demand is more and more satisfied by an inflow from outside r = 8000 ft, rather than from storage inside this region. This explains the observed delay in the propagation of the transition radius.

Given the limitations of the finite element grid used in this particular test, AQUIFEM-1 performs remarkably well. It should be kept in mind however, that AQUIFEM-1 is not designed specifically for handling *moving boundary problems;* in fact, the options for handling the change of status problem are rather heuristic and are aimed at providing qualitative rather than quantitative results. Similar comments can be made about other models of this type (e.g., Prickett and Lonnquist, 1971). The design of numerical methods for solving moving boundary problems is still an area of active research in many fields of application. Recent work in the field of heat flow and diffusion (melting, solidification and Stefan problems) can be found in Ockendon and

Hodgkins, 1975. In a groundwater application, Sa da Costa and Wilson (1979) describe a method for tracking the toe of a seawater wedge in coastal aquifers.

5.3 Summary

The test cases presented above have demonstrated the ability of AQUIFEM-1 to produce good approximate solutions to a variety of groundwater problems. Extremely good accuracy is achieved for all the one-dimensional problems, both linear and nonlinear, steady and unsteady, the good results being attributable to the use of a regular grid and the inherent abilities of the finite element method. In order to simulate situations with radial symmetry, finite element grids with a continuous gradation in element size are used, thus illustrating one of the advantages of the finite element method. The numerical solutions for pumping from leaky and nonleaky confined aquifers compare very well with analytical solutions, at the same time pointing out the need for care in accurately representing boundary conditions. The solution for pumping from a well with a progressive transition from confined to unconfined behavior agrees qualitatively with the exact solution, however, care should be exercised when studying this behavior in practical applications; the results are pleasing considering the fact that the model is not specifically designed for this difficult class of problems.

In conclusion, AQUIFEM-1 can successfully model many types of groundwater problems. Only a fraction of the model's capabilities are demonstrated here, all programming options being described in

detail by Townley and Wilson, 1980. It is believed that AQUIFEM-1 satisfies all the objectives outlined in Section 1.2 of this report and that it will provide a useful tool for groundwater managers in the future.

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APPENDIX A

LIST OF SYMBOLS

A (i) Area of a finite element

(ii) Amplification factor in finite difference analysis

$\mathcal{A}(\ )$ Assembly operator

a Dimensionless parameter in analysis of leaky aquifer, equal to $(K'/B'K_{xx}B)^{1/2}$

a_i Coefficients in polynomial representation of interpolation functions

B Aquifer thickness

B' Thickness of adjacent semipervious layer

B" Effective depth (parallel to a leaky flow) of leaky zone on Γ_3

b_i Coefficients in polynomial representation of interpolation functions

C,C* Constants

c_i Coefficients in the polynomial representation of interpolation functions

$\underline{e}$ Vector of errors or deviations between exact and approximate solutions

F An arbitrary function

f A function related to known distributed or point fluxes and leakage

$\underline{f}$ Vector related to known boundary values, fluxes and leakage

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$\underline{f}^e$	Element contribution to $\underline{f}$
f_i	Component of $\underline{f}^e$ or $\underline{f}$
$\underline{f}^e_{AQUIFEM-1}$	Form of element flux vector used in AQUIFEM-1 computer code
$\underline{\underline{G}}$	Matrix relating $\underline{h}$ and $\underline{\alpha}$
$\underline{g}$	Vector of known heads at nodes on Γ_1
g_j	Component of $\underline{g}$ at $j\underline{th}$ node
h	Depth averaged piezometric head
h_1	Known piezometric head on Γ_1
$\underline{h}^*$	Vector of nodal values of h (exact values)
$\hat{h}$	Assumed approximate distribution of h
$\underline{h}$	Vector of nodal values of $\hat{h}$
h_i, h_j	Components of $\underline{h}$ at $i\underline{th}$, $j\underline{th}$ nodes
h_a	Depth averaged piezometric head in an adjacent aquifer
$h_{a,i}$	Value of h_a at $i\underline{th}$ node of an element
h_o	(i) Known initial value of h at time t_o (ii) Known value of h at $x = 0$
h_L	Known value of h at $x = L$
h_3	Known piezometric head beyond leaky zone on Γ_3
$h_{3,i}$	Value of h_3 at $i\underline{th}$ node of an element
h_n	Approximation to $h(t_n)$ in finite difference solution of a single-degree-of-freedom problem
$\underline{h}_n$	Approximation to $\underline{h}(t_n)$ in finite difference solution of the aquifer finite element equations

$\tilde{\underline{h}}_{n+1}$	Vector of known information at the start of (n+1)th time step--equal to $(\underline{h}_n + (1-\alpha)\Delta t\ \underline{v}_n)$
$\vec{i},\vec{j}$	Unit vectors in the x,y directions
K	Depth averaged hydraulic conductivity (permeability)
K_{xx},K_{yy}	Values of K in x,y directions
K_{rr}	Value of K in radial direction
K'	Vertical hydraulic conductivity of an adjacent semipervious layer
K"	Equivalent hydraulic conductivity of leaky zone on Γ_3
$\underline{\underline{K}},\underline{\underline{K}}^*$	Matrices of coefficients which depend on aquifer transmissivities, leaky layer properties and geometry of the finite element grid
k	(i) Degree of highest order polynomial which can be exactly represented by given interpolation functions (ii) Order of accuracy or rate of convergence of finite difference time integration algorithm
$\underline{\underline{k}}^e$	Element contribution to $\underline{\underline{K}},\underline{\underline{K}}^*$
k_{ij}	Component of $\underline{\underline{k}}^e$, $\underline{\underline{K}}$ or $\underline{\underline{K}}^*$
$\underline{\underline{k}}_3$	Contribution to $\underline{\underline{k}}^e$ due to an element side on Γ_3
$\underline{\underline{k}}^e_{AQUIFEM-1}$	Form of element conductivity matrix used in AQUIFEM-1 computer code
L	(i) Measure of the length of a finite element (ii) Length of a one-dimensional aquifer
L( )	A linear differential operator

$\underline{M}, \underline{M}^*$	Matrices of coefficients which depend on storativities and grid geometry
$\underline{m}^e$	Element contribution to $\underline{M}, \underline{M}^*$
$\underline{m}^{e*}$	Alternative form of $\underline{m}^e$ using mass lumping
$\underline{m}^e_{AQUIFEM-1}$	Form of element storage matrix used in AQUIFEM-1 computer code
m_{ij}	Component of $\underline{m}^e$, etc.
m	Order of highest derivative in the weak form of the boundary value problem
N_i, N_j	Interpolation functions defined for ith, jth nodes
$\underline{N}$	Vector of element interpolation functions
$\vec{n}$	Unit inward pointing normal vector on the boundary
n_x, n_y	Components of $\vec{n}$ in x,y directions
p	Arbitrary index
$\underline{p}$	Vector used in Cartesian analytical geometry
Q	Net vertical flux from point or distributed sources*
Q_e	Uniform vertical flux distributed over an element*
Q_n	Point vertical flux at a node*
Q_s	Known horizontal flux per unit width on Γ_2*
Q_x	Horizontal flux per unit width in the aquifer in the x direction
q	Arbitrary index
R	Radius at which conversion from confined to unconfined behavior is taking place in Test Case 9

*All these fluxes are positive into the aquifer.

r	(i)	Radial coordinate direction
	(ii)	Arbitrary index
	(iii)	Measure of the length of a finite element
S		Aquifer storage coefficient
S_o		Specific storativity
S_y		Specific yield
s		Length of an element side
T		Aquifer transmissivity
T_{xx}, T_{yy}		Transmissivities in x,y directions
T_{rr}		Transmissivity in radial direction
$t, \Delta t$		Time, increment of time
t_o		Time at which initial conditions are known
t_n, t_{n+1}		Times of $n\underline{th}$, $(n+1)\underline{th}$ time steps
u		Rate of convergence of the finite element method in space
$u, u_1, u_2,$ v_1, v_2		Dimensionless parameters in well analysis of the form $(r^2S/4Tt)$
$\vec{v}$		Arbitrary vector-valued function
v_x, v_y		Components of $\vec{v}$ in x,y directions
v		Alternative notation for $\dot{h} = \partial h/\partial t$
v_n		Approximation to $\dot{h}(t_n)$
$\underline{v}_n$		Approximation to $\underline{\dot{h}}(t_n)$
W''		Effective width (perpendicular to leaky flow) of leaky zone on Γ_3
$W(u)$		Well function for nonleaky aquifers

$W(u,r/b)$	Well function for leaky aquifers
w, w_i	Weighting functions in derivation of the finite element method
w_n	Weighting coefficient for determining contribution of Q_n to $\underline{f}^e$
w_2	Weighting coefficient for determining contribution of Q_s to $\underline{f}^e$
w_3	Weighting coefficient for determining contribution of $(K''W''/B'')h_a$ to $\underline{f}^e$, $\underline{k}_3$
$X(x/L)$	Function defining initial conditions in Test Case 8
x,y	Cartesian coordinates (principal directions)
x_i, y_i	Coordinates of i<u>th</u> node of a triangular element
z	Aquifer bottom elevation
α	Parameter of a family of time integration schemes
α_i	Coefficients in polynomial representation of a plane
$\underline{\alpha}$	Vector with components α_i
β	Dimensionless parameter in analysis of leaky aquifers, equal to $(B'T/K')^{1/2}$
Γ	Boundary of the aquifer domain
Γ_1	1st-type boundary segment
Γ_2	2nd-type boundary segment
Γ_3	3rd-type boundary segment
Γ^e	Boundary of a finite element
$\vec{\nabla}$	Gradient operator in vector calculus

λ Coefficient in single-degree-of-freedom problem for studying finite difference analysis

λ_i Eigenvalue corresponding to ith unknown in system of linear equations

λ_{max} Largest eigenvalue in a system of linear equations

Ω Domain of an aquifer or solution domain of a partial differential equation

Ω^e Element domain

ϕ Depth averaged piezometric head in a confined aquifer

ϕ_a Depth averaged piezometric head in an adjacent confined aquifer

ϕ_o (i) Known initial value of ϕ at time t_o
(ii) Known value of ϕ at $x = 0$

ϕ_L Known value of ϕ at $x = L$

ϕ_3 Known piezometric head beyond a leaky zone on Γ_3

$\underline{\Psi}_i$ Eigenvector corresponding to λ_i

τ Local truncation error in a finite difference solution

Subscripts:

$(\ )_o$ Quantities evaluated at the initial time t_o

$(\ )_n$ Quantities evaluated at the nth time step

$(\ )_\ell$ Quantities for the ℓth element

Superscripts:

$(\ )^T$ Matrix transpose

$(\ )^{-1}$ Matrix inverse

$(\ )^{(i)}$ Quantities evaluated after ith iteration

$(\dot{\ })$ Time derivative of a quantity

FORTRAN variable names from AQUIFEM-1 computer code*

DTPARM A multiplicative factor by which the time step increases after every NDT time steps. (In all Test Cases in this report, NDT = 1.)

ITOL Indicate the method by which convergence is tested. If ITOL = 0, the root mean square error is used; if ITOL = 1, the maximum absolute deviation is used.

MAXIT Maximum number of iterations considered reasonable in a given time step. Normally if MAXIT is exceeded, the program stops, however, if a change of status has occured in that time step, the program continues to the next time step.

NEQ Number of equations,equal to the number of nodes where the head is unknown.

NSYS Number of iterations between updating the left-hand-side system matrix.

NUMEL Number of elements in the finite element grid.

NUMNP Number of nodal points in the finite element grid.

TOL Tolerance for testing convergence.

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*See Townley and Wilson, 1980.