AN INVERSE PROBLEM IN AQUIFER PARAMETER IDENTIFICATION

C.R. Dietrich, F. Ghassemi and A.J. Jakeman

1. Introduction

By definition an aquifer is a formation that contains sufficient saturated permeable material to yield significant quantities of water to wells and springs. Aquifers, or water-bearing formations, can be characterised largely by two parameters: the storage coefficient S and the transmissivity T .

The storage coefficient is defined as the volume of water that a vertical column of aquifer with a unit area will release or take up if the piezometric surface changes by one unit. The coefficient is dimensionless involving a volume of water per unit volume of aquifer.

The transmissivity of an aquifer is defined to be the product of its thickness b by its hydraulic conductivity k , viz.

$$T = kb \quad . \tag{1}$$

As the dimension of k is $[LT^{-1}]$, the dimension of transmissivity is $[L^2T^{-1}]$.

Any project for development of groundwater resources in a given region requires a good knowledge of the aquifer's quantitiative and

qualitative properties. Moreover, it is important to be able to predict the effect of groundwater development schemes (such as drilling of new bores, artificial recharge, etc.) on the behaviour of the aquifer.

Powerful tools for achieving the above objectives are mathematical groundwater models based on solution of the following partial differential equation (e.g. Bear, 1972) representing two-dimensional transient flow in a confined aquifer

$$(2) \qquad \frac{\partial}{\partial x}\left[T\frac{\partial \varphi}{\partial x}\right] + \frac{\partial}{\partial y}\left[T\frac{\partial \varphi}{\partial y}\right] = S\frac{\partial \varphi}{\partial t} + q(x,y,t) \ .$$

Here x and y are the cartesian coordinates and t is time, while T is transmissivity and S is the storage coefficient (both of which tend to be largely unknown except for some point estimates), φ is the hydraulic head (which is known reasonably well spatially), and $q(x,y)$ is the source or sink term (some component of which may be known).

Equation (2), with T and S as the dependent variables, is often termed the aquifer identification (AI) problem. It is clear that to set up a mathematical model of aquifer behaviour an accurate distribution of these values is required. However, in most cases these distributions are not available and mathematical modellers tend to use a trial and error technique, involving tests of the effect of different distributions of T and S on the computed piezometric heads to get the best possible match between measured and computed values. Such trial and error techniques are very time consuming and their accuracy depends on the accuracy of the other data supplied. Thus during the

last decade attention has been given largely to the development of techniques for more explicit solution for the parameters in the AI problem (2), and to determination of the properties of resultant approximations and their dependence on the form of the input data.

It is instructive to describe the particular aquifer and associated problems with which we are presently dealing in the Mildura-Merbein area, as well as some of our results using the trial and error technique. The River Murray Basin is a large shallow basin filled by Tertiary and Quaternary sediments, resting uncomformably on a basement of mainly Palaeozoic sedimentary and crystalline rocks. This sedimentary basin contains, from bottom to top, the following major aquifers: Warina sand of Paleocene-Eocene age, Duddo limestone of Oligocene-Miocene age, and Parilla sand of Pliocene age. In the Mildura-Merbein area only the Parilla sand aquifer has been simulated (Ghassemi et al, 1986), as accurate information regarding the deep aquifers is unavailable. This necessitated simplification of the model to a two-dimensional structure. The dimensions of the study grid were chosen to give a discretisation step of 200m, yielding 40 x 31 modes. Due to the geometry of the aquifer about 800 of these are active.

Piezometric measurements in the Mildura-Merbein area commenced in 1967 in 15 locations. These measurements ceased in July 1968 and resumed in November 1970. More piezometers were installed in three subsequent periods: 1970, 1973 and 1979-80. Now there are more than 150 piezometers in this area. Most of the piezometers are located adjacent to the River Murray, but there is also a small percentage of piezometers scattered sparsely throughout the remainder of the study area.

Piezometric measurements before 1980 are temporally sparse and gaps of a few years in the records are not unusual. However, from the end of 1979 measurements became more regular and more reliable. Thus the period from January 1980 to March 1983 was selected for piezometric data analysis and for calibration of our mathematical models on the basis of the accuracy of piezometric data and their good correlation with hydrographic measurements.

Figure 1 is a stylised map of the Mildura-Merbein study area showing piezometric contours for the month of January in 1980. Piezometric maps for this and other months show that: (a) the piezometric heads of the aquifer range from over 38m to about 31m in transects from south to north; (b) the hydraulic gradient is steeper close to the River rather than in the south; (c) the River Murray is the discharge zone of the aquifer; and (d) the closed contour lines of 36m and above on the north east of Lake Ranfurly are due to irrigation. With a contour map of the area, the piezometric values can easily be converted to groundwater depth. The groundwater depth map of January 1980 shows that in general the piezometric level of the aquifer is more than three metres deep with a maximum depth of about eight metres between Lake Ranfurly and the Murray.

It will be shown in Section 2 how pumping tests can be used to obtain point estimates of T and S values. The results of pumping tests carried out in 1973 on the Mildura aquifer have been reported by the State Rivers and Water Supply Commission of Victoria. Here the transmissivity values range from 80 to 500m^2/day and storage coefficient values vary from 0.001 to 0.05.

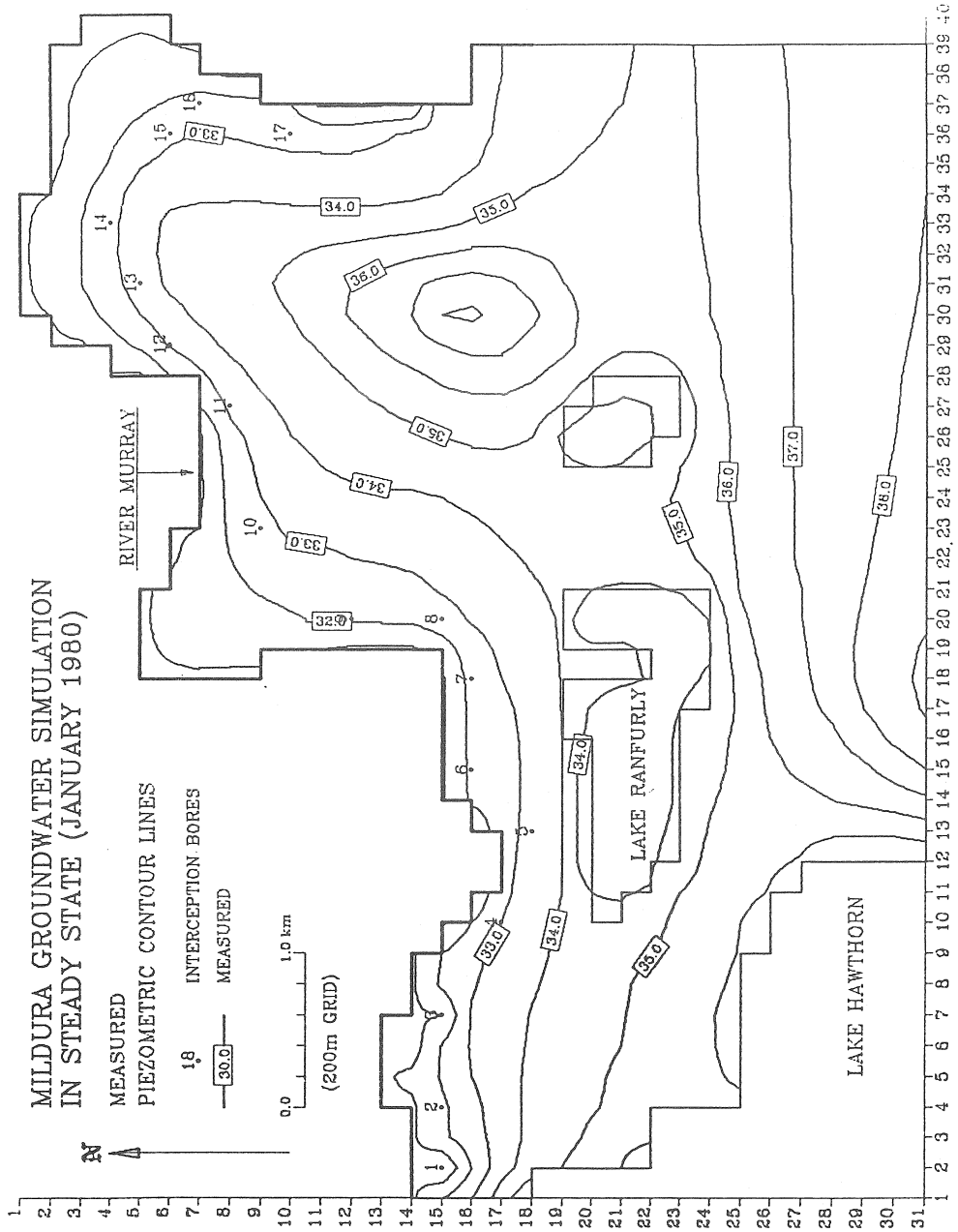

Figure 1. Measured Piezometric contour lines of the Mildura aquifer in January 1980.

More recent measurements of T values provided by the Rural Water Commission of Victoria indicate higher values of T with a maximum of $1300 m^2/day$. It should be noted that in both cases all measurements have been performed in the northern part of the aquifer adjacent to the river. Figure 2 shows the location of transmissivity point measurements. The poor spatial distribution of T and S measurements and doubt about their accuracy have been major problems in the calibration of mathematical models of the Mildura aquifer.

Other data required for calibration of the T and S values in the groundwater flow model in the Mildura-Merbein area include: boundary conditions and recharge estimates and discharge rates (the q term). The Murray and the Lakes (Ranfurly and Hawthorn, shown in Figure 1) were simulated as fixed head boundaries; the eastern boundary not covered by the Murray is a non-flow boundary; and the southern and western boundaries are inflow boundaries. Daily rainfall and monthly irrigation data were used to develop recharge estimates. During the model calibration the rate of percolation was estimated to be 5% of rainfall for the city area, 10% of rainfall for the rural areas, 20% of irrigation supply for vineyards and citrus orchards, and 40% of irrigation for pastures. The remainder is considered to be used by plants, drained by tile drainage or evaporated from the soil surface. Significant leakage from a lagoon was also found; this was estimated during the model calibration phase. Discharge in the form of withdrawal from interception bores is well measured and does not require estimation.

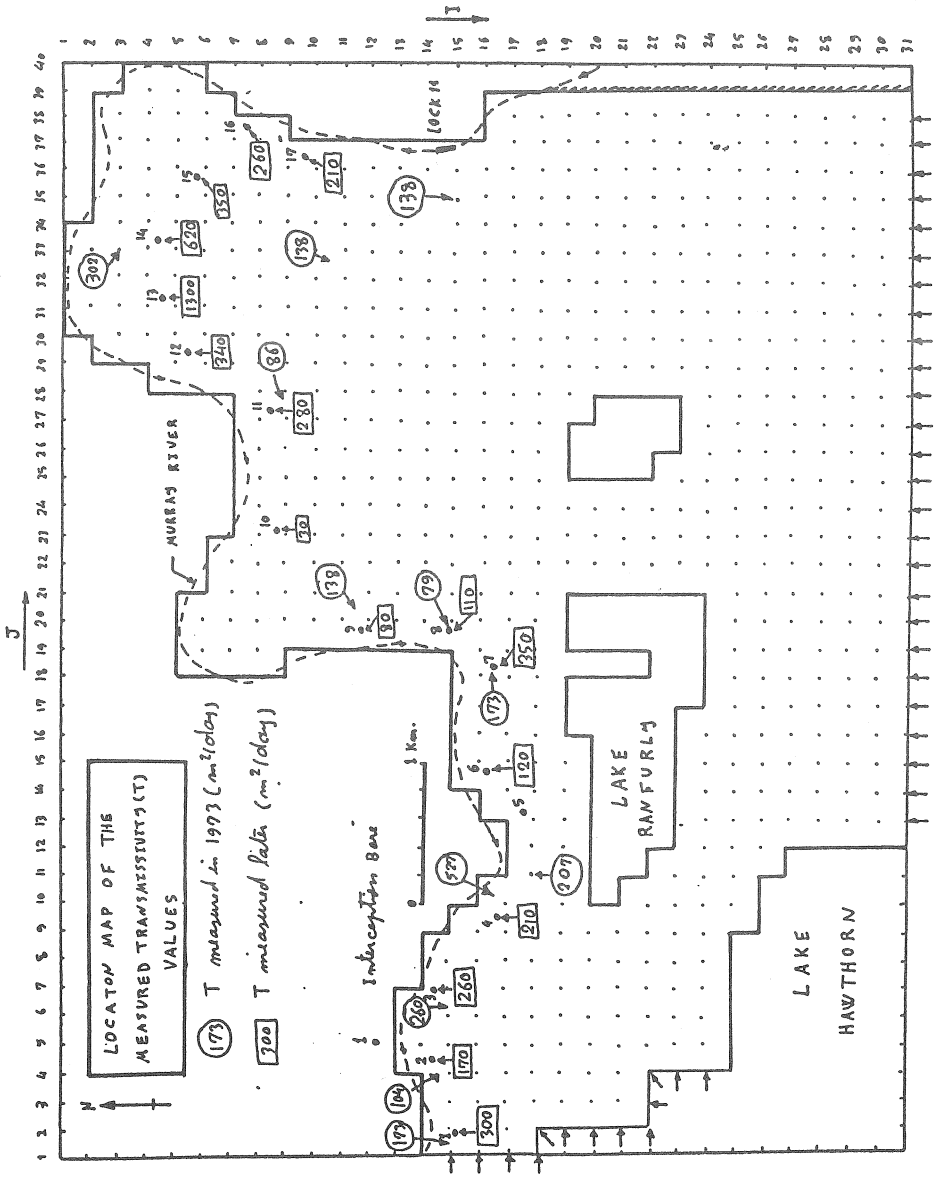

Figure 2. Location map of transmissivity point measurements.

In summary, the model calibration involves not only estimation of T and S values, but also of recharge rates and boundary conditions. However prior data and hydrogeological knowledge helps to pin down candidate parameter values. Therefore information is available on all variables but the precision of such information varies widely with the variable and the location. For example, φ , T and S estimates are available in some areas, only φ in some others, while in some there is no information about any. Thus in the AI problem φ is classified as data while T and S are classified as unknowns simply because more information is available on φ than on T and S . In practice the problem is rather to use the given data on φ , T , S and q together with the model in equation (2) of flow in an aquifer to extrapolate φ , T and S across the entire aquifer.

Unfortunately this problem is effectively intractable in its full generality. Therefore the paper will concentrate on the special case of steady-state flow, i.e. on the case when inflows and outflows to and from the aquifer balance so that

$$\frac{\partial}{\partial t}\varphi(x,y,t) = 0 \qquad \forall\, x,y \ .$$

In this case the parameter S vanishes from (2) and only φ and T are to be determined. Note that it is not necessary that $\partial\varphi/\partial t$ vanish identically for all time in order to derive a steady state problem. For example, if the aquifer displays some sort of cyclic behaviour, e.g. on an annual basis, so that

$$\varphi(x,y,t) = \varphi(x,y,t+1)$$

then

$$\int_t^{t+1} \frac{\partial \varphi}{\partial t} = 0$$

and (2) becomes

$$\left[\frac{\partial}{\partial x}\left[T\frac{\partial}{\partial x}\right] + \frac{\partial}{\partial y}\left[T\frac{\partial}{\partial y}\right]\right]\int_t^{t+1} \varphi \, dt = \int_t^{t+1} q(x,y,t)dt \ .$$

To conclude the introduction, we provide some results using the trial and error method with constant zonation for solving (2) for T. Figure 3 shows the calibrated T values for the Mildura aquifer in steady-state. The φ data used are those contoured in Figure 1 for January 1980. Note that transmissivity has been assumed constant in five different zones. The zones were chosen on the basis of hydrogeological knowledge and hypothesis testing using the trial and error technique. Thus a distribution of T values is assumed and then (2) is solved for φ, this is the forward problem. The agreement between measured and computed φ is then assessed and, if necessary, a new distribution of T values is hypothesised followed by a further solution of the forward problem. This process continues until satisfactory agreement has been obtained for φ together with a solution for T consistent with the known hydrogeological properties and behaviour of the aquifer. Figure 4 shows the relationship between measured and computed φ values for the steady-state case in January 1980.

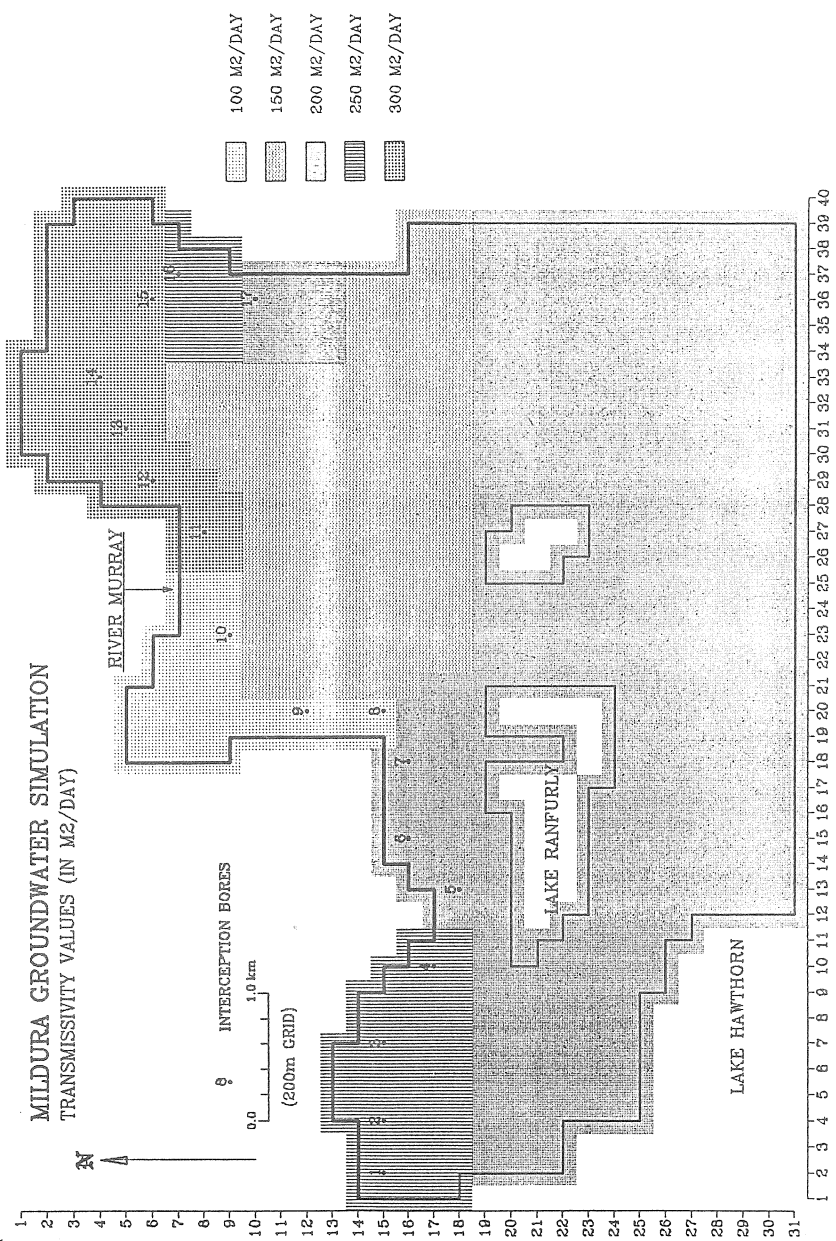

Figure 3. Distribution of calibrated transmissivity values.

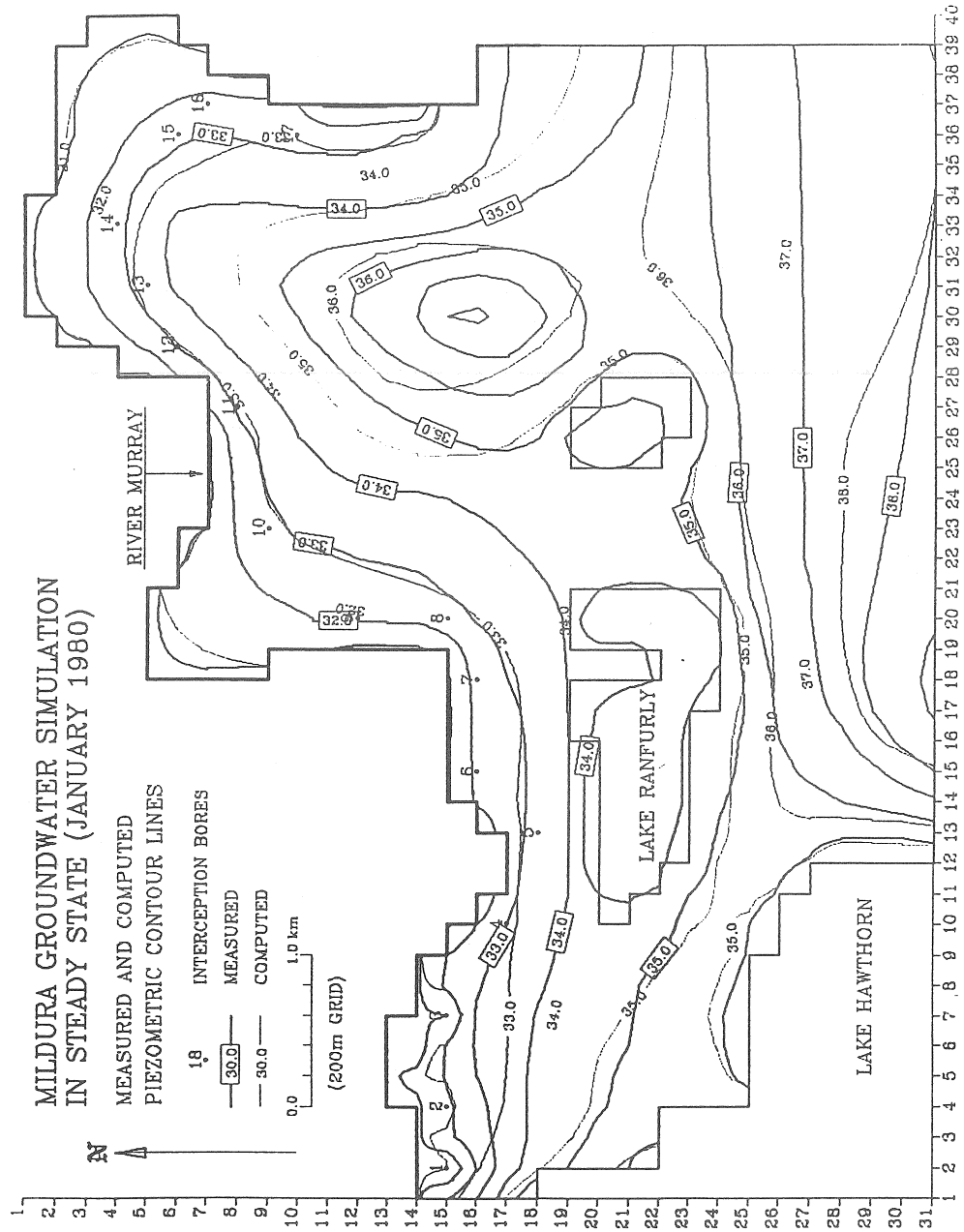

Figure 4. Measured and computed Piezometric contour lines of the Mildura aquifer in January 1980.

The remainder of the paper is as follows. In Section 2 it is seen how T and S can be measured in practice. Section 3 examines the form of the inverse problems considered here in particular the problem of estimating T from a steady-state model. A cursory review of the literature is presented in Section 4. Section 5 illustrates the importance of low parameterisation in providing a unique and stable solution to AI. Tikhonov regularisation is discussed in Section 6. In Section 7 we examine the merits and drawbacks of the geostatistical approach. Section 8 contains the conclusions and in particular notes a method being presently explored as a result of discussion at the workshop.

2. Measurement of T and S values

The technique for measurement of T and S from pumping tests (see Figure 5) is based on the solution of a partial differential equation of unsteady radial flow in a confined aquifer (Todd, 1980). The equation is

$$\frac{\partial^2 \varphi}{\partial r^2} + \frac{1}{r}\frac{\partial \varphi}{\partial r} = \frac{S}{T}\frac{\partial \varphi}{\partial t} \tag{3}$$

in which

- φ is the piezometric head of the aquifer;
- r is the radial distance of the observation well from the pumped well;
- S is the storage coefficient (assumed constant);
- T is the transmissivity (assumed constant);
- t is time .

Theis (1935) provided a solution for (3) under a few assumptions including the following: the aquifer is homogeneous, isotropic of uniform thickness and of infinite extent; before pumping the piezometric surface is horizontal; the well is pumped at a constant discharge rate Q ; the pumped well penetrates the entire aquifer; and flow within the aquifer is everywhere horizontal to the well. The solution is:

$$s = \frac{Q}{4\pi T} \int_u^\infty \frac{e^{-\xi} d\xi}{\xi} \tag{4}$$

where

s is the drawdown (this is a simple function of C);

Q is the constant well discharge;

and

$$u = \frac{r^2 S}{4Tt} . \tag{5}$$

The integral in (4) can be expanded as a convergent series so that the equation becomes

$$s = \frac{Q}{4\pi T} \left[-0.5772 - \ln u + u - \frac{u^2}{2.2!} + \frac{u^3}{3.3!} - \frac{u^4}{4.4!} + \ldots\right] \tag{6}$$

or

$$s = \frac{Q}{4\pi T} W(u) \tag{7}$$

where $W(u)$ is known as the well function and whose values are tabulated in most hydrogeological handbooks (Freeze, 1979 and Todd, 1980).

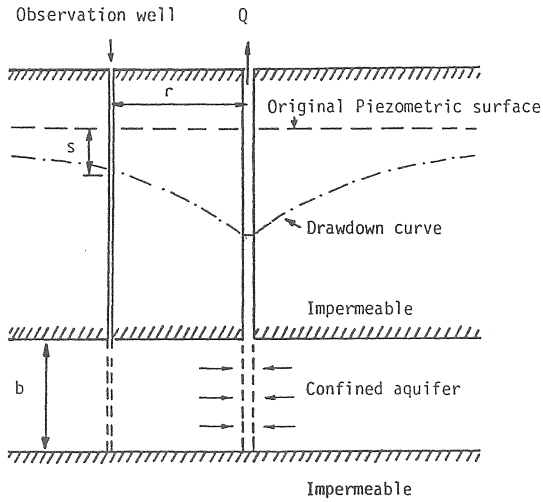

Figure 5 Pumping test in a confined aquifer

In practice, during the pumping test the drawdown s is an observation well at a distance r from the pumping well is measured at different times t. On the basis of the s, t and r values, a plot is constructed of s versus r^2/t on a logarithmic scale. Values of $W(u)$ and u are also plotted on a logarithmic scale. The two sheets are superimposed and shifted with coordinate axes parallel until the observation point coincides with the curve of $W(u)$ versus u. Then an arbitrary match point is selected. Reading the coordinates of the match point on both logarithmic graphs (see Figure 6) yields 4 values of s, r^2/t, u and $W(u)$. Substitution of these 4 values in the following equations (derived from equations (7) and (5) respectively) provides T and S values for the aquifer in the region of influence of the pump test, with

$$T = \frac{QW(u)}{4\pi s}$$

$$S = \frac{4Tu}{r^2/t} .$$

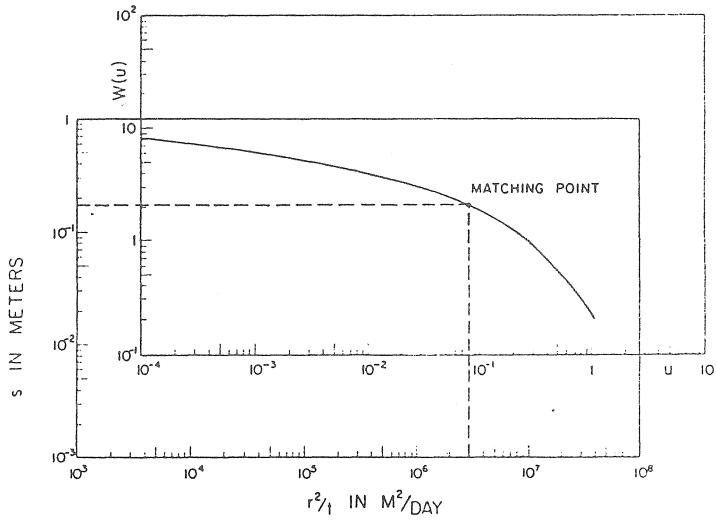

Figure 6 Superposition of two plots to obtain coincident curves and selection of match point (after Bouwer, 1978).

Pumping tests are time consuming and expensive. Therefore it is not practical to use them extensively for the measurement of transmissivity and storage coefficient values in different parts of the aquifer. In practice, hydrogeologists use prior knowledge of the aquifer's geology to try to extrapolate measured values through the whole aquifer.

3. Inverse aquifer identification problems

Here attention is restricted to the steady-state, 2 dimensional flow equation for a confined, isotropic and non-homogeneous aquifer. In this case the governing PDE (2) linking the piezometric head φ ,

transmissivity T and sink term q can be concisely written as

$$\nabla \cdot (T\nabla\varphi) = q \quad \text{on} \quad \Omega \tag{8}$$

subject to appropriate boundary conditions on $\partial\Omega$. Here ∇ denotes the gradient operator, $\cdot$ an inner product, and Ω the flow domain with boundary $\partial\Omega$.

Let us first mention the forward problem which amounts to solving (8) for the dependent variable φ given models for T and q as well as Dirichlet and/or Neumann boundary conditions for φ on $\partial\Omega$. This formulation represents an elliptic PDE for the head φ. It is well known (Courant and Hilbert, 1962) that given appropriate boundary conditions the solution of elliptic PDE's is a properly posed problem. As well as guaranteeing existence and uniqueness, this implies that φ depends continuously on T and q. As a consequence, methods for solving the forward problem are straightforward (Pinder and Gray, 1977).

Turning attention to the inverse problem, its exact form depends on whether it is only T, T and q, or any combination of T, q and boundary conditions, which are the unknowns. Consequently, rather than a single problem, one has a variety of inverse problems for which different methodologies must be developed in order to fully utilize the information contained in the available data. In fact it is essential to ascertain that for a given form of AI the data contain sufficient information to, at least in principle, yield a unique and meaningful solution. In this paper we shall examine the standard AI problem where T is the major unknown and the following information is given

I head measurements φ_i $i = 1,\ldots,I$;

Dirichlet and/or Neumann boundary conditions for φ ;

J transmissivity measurements T_j $j = 1,\ldots,J$

with $J << I$;

a model of the sink term $q(x,y)$, $(x,y) \in \Omega$.

This AI problem amounts to deriving a model for $T(x,y)$ so that solution of the PDE (8) yields a function $\varphi(x,y)$ that fits the piezometric head data φ_i in some optimal way. This of course will involve a trade-off between fidelity to the φ_i data and the construction of a realistic solution $T(x,y)$.

4. Cursory review of the literature

Neuman (1979) has provided a classification of AI methodologies into direct and indirect methods. Upon discretisation of the aquifer, direct methods reduce (8) to the matrix equation

$$\mathbf{AT} = \mathbf{b} + \boldsymbol{\epsilon}$$

where $\mathbf{A}$ is a known matrix function of φ_i , $\mathbf{T}$ is the unknown vector containing transmissivity values at each node of the grid, $\mathbf{b}$ is a known vector funtion of φ_i and q , and $\boldsymbol{\epsilon}$ is a residual term representing water mass balance errors at each node of the grid. The transmissivity is then estimated by linear least squares procedures. The estimation procedure is computationally simple. It is, however, unstable in the presence of noise in piezometric head measurements.

On the other hand, indirect approaches solve the forward problem for $\varphi(T)$ iteratively. The error in history matching for φ can be written in matrix form as

$$C\varphi = (\varphi_h) + \mathbf{n}$$

where C is a matrix containing the unknown transmissivity values; φ is the dependent vector of piezometric head; (φ_h) is the vector of observed piezometric heads; and $\mathbf{n}$ is a vector of history matching errors. The transmissivity is then estimated by minimising the output error $\mathbf{n}$. This requires non-linear least squares estimation since φ is not a linear function of T. The search for a minimum is usually performed by gradient-type methods (Cooley, 1977, 1982; Neuman, 1980) or control-oriented techniques (Chen et al., 1974; Chavent et al., 1975). This approach is basically stable, but uniqueness of the solution cannot be guaranteed when noise in the data causes the error surface to be non-convex. Thus the solution may depend strongly on the initial estimates of the parameters. In addition the indirect approach is computationally expensive, although highly efficient algorithms based on the adjoint state theory of Chavent (1971, 1975) and reported in Neuman (1980) have considerably reduced the computer time allocated to gradient estimation.

It is worth mentioning that most methods reported in the literature, whether direct or indirect, set the AI problem within a deterministic framework and statistical tools are used only to process error terms. For more details the reader is referred to Yeh (1986) who provides a very thorough and comprehensive updated review of the deterministic methodologies.

Compared with deterministic techniques, stochastic approaches are somewhat new and less well documented. Bastin (1981) treats the one-dimensional case and provides an estimator for the transmissivity by assuming it to be a random walk in space. However, his method cannot be extended to two dimensional problems. Yakowitz (1976) uses methods from clustering and time series analysis to provide a model-free estimation of parameters. Vomvoris (1983), Hoeksema and Kitanidis (1984) and Dagan (1985) use concepts borrowed from the theory of random fields (Wiener and Masani, 1958; Matheron, 1973) to develop the so-called geostatistical approach to the AI. In this direct methodology, the unknown transmissity is assumed to be random so that its identification reduces to deriving a stationary structure which is linear in the parameters for the mean (also called the drift) and the covariance. Under certain ergodic assumptions about the unknown transmissivity (Papoulis, 1964) a maximum likelihood estimation of the parameters can be carried out directly with use of the whole data set, assuming that the sample distribution of transmissivity is lognormal (Bakr et al., 1978).

The geostatistical approach is intuitively appealing in that it recognises that the transmissivity can only be known in a statistical sense. In addition, the assumed form of the covariance structure stabilizes the problem and the method automatically chooses an appropriate stabilization parameter (q.v. Sections 5 and 6 below). Thus the method always determines a unique solution even when only a relatively small amount of independent data is available.

However there are a number of drawbacks in the method as proposed in the literature. In order to avoid large nonlinear optimization problems the determination of parameters by maximum likelihood estimation is broken up into several stages. The approximations needed to carry this out may lead to inconsistent problems if care is not taken, and may also be so severe as to vitiate the method. For example, a recent implementation by Kuiper (1986) performed no better than a simple indirect algorithm. These points are discussed further in Section 7.

5. Mathematical structure of the AI problem

Equation (8) is a first order hyperbolic equation in the dependent variable T. Its continuous solution (see Appendix A) over any characteristic Γ defined by $\nabla h = (dx/d\theta\ ,\ dy/d\theta)$ is

$$T(\theta) = \psi(\theta)\left[\int_0^{\theta}\frac{q(\eta)d\eta}{\psi(\eta)} + c\right] \tag{9}$$

where $\psi(\eta) = \exp\left[-\int_0^{\theta}\Delta\varphi(\xi)d\xi\right]$, c is a constant and Δ denotes the Laplacian operator.

Equation (9) shows that the solution for T exists and is unique along a characteristic Γ if and only if $\Delta\varphi \not\equiv 0$ and there is exactly one piece of information about T so that the constant c is determined uniquely. This means that T exists and is unique in Ω provided a value of T, the so-called Cauchy data, is known on each characteristic in Ω. The following points can now be deduced directly from the structure of equation (9):

(5.1) In the absence of transmissivity data the solution for T is not uniquely determined, even though φ and q may be known exactly.

(5.2) Even when T exists and is unique it does not depend continuously on the piezometric head data since T is defined in terms of derivatives of φ. In other words, small errors in measurements of φ may be magnified in $\nabla\varphi$ and thereby lead to unstable estimates of T.

(5.3) T depends continuously on q and on c, i.e. small errors in q and T data yield only small errors in estimates of T.

(5.2) shows that the inverse problem of AI is only mildly improperly posed in that it corresponds to one differentiation of the head φ. The improperly posedness of (5.1) and (5.2) resulting from the structure of equation (9) is still present when the aquifer is discretised and the transmissivity is parameterised. To illustrate this important point, assume a finite parameterisation of the transmissivity T viz.

$$T(x,y) = \sum_{n=1}^{N} \tau_n v_n(x,y) \tag{10}$$

where the $v_n(x,y)$ are known independent basis functions and the τ_n are the associated unknown coefficients. AI then amounts to estimating the N parameters τ_n. Providing there are N independent pieces of information in the data base, in principle a unique solution for τ_n can be computed even though no transmissivity data are available at all.

However, the solution obtained via such a simple algebraic method is very unstable. Therefore, in the presence of small errors in head measurements realisations of the true solution are likely to show large oscillations and are therefore unacceptable.

An obvious stabilisation technique is to reduce N and derive a solution for the overdetermined algebraic system, say, by least square procedures. At the limit $N = 1$ (e.g. T being assumed constant over the whole aquifer,) the ill-posedness of the discrete AI is completely removed. This obviously is done at the cost of the degree of resolution of transmissivity estimation. This is a typical feature of stabilisation; a trade-off must be made between the degree of numerical ill-posedness and the resolution of the estimated transmissivity. Therefore one has to forgo accuracy in estimates of T in order to decrease the degree of ill-posedness. Note that in the frequency domain this feature is equivalent to the suppression of high harmonics in estimates of T (Allison and Peck, 1985).

Thus a fundamental question in discrete AI is the search for optimum N and basis functions $v_n(x,y)$. This question has been addressed in several papers (Sun and Yeh, 1985); due to the intrinsic mathematical difficulties satisfactory answers have yet to be found.

6. Tikhonov regularisation

In the search for a practically useful solution to AI the choice of an adequate stabilisation procedure is essential. Apart from maintaining a low parameterisation for the transmissivity T some

authors in their formulation add to the norm of the model errors a norm of the form $\lambda\|T-T^*\|$, where T^* is determined by prior transmissivity data and λ is the regularisation parameter. The norm itself may be weighted by the inverse of a covariance matrix for T when prior knowledge about the system allows such a matrix to be derived (Carrera and Neuman, 1986). It should be noted that the estimation procedure for obtaining an optimal value for λ as well as the rigorous derivation of statistical properties of the errors is far from obvious when an indirect approach is used. The principal reason is that such a procedure involves non-linear regression. On the other hand, while direct approaches are amenable to linear regression, the approximations generated are unstable in the presence of piezometric head measurement noise.

An interesting approach to stabilisation reported in Allison and Peck (1985) is Tikhonov regularisation. Suppose we wish to solve $Lu = q$ for u with L assumed to be a bounded linear operator. If L has an unbounded inverse, a regularised solution u_λ is sought by minimising

$$\|Lu - q\|^2 + \lambda\|Pu\|$$

where λ is the regularisation parameter and P is a linear differential operator. Under rather general conditions theorems on the existence and uniqueness of u_λ may be derived (Kravaris and Seinfeld, 1985) and an optimum choice of basis functions for T made (Lukas, 1980).

Again, the regularisation approach involves a trade-off between accuracy and stability of the solution of the improperly posed problem. Here, it is determined by the weight λ . When its value increases, the solution becomes more stable but less accurate. So far Tikhonov regularisation does not seem to have been used for aquifer identification via direct approaches. Its potential justifies further investigations.

7. The geostatistical approach to AI: Merits and drawbacks

Among direct methods for the inverse problem in aquifer identification is a relatively new geostatistical approach reported with two dimensional case studies in Hoeksema and Kitanidis (1985) (see also Kuiper (1986)). However Dietrich et al (1986) have found that the methodology as proposed has a number of flaws. In order to clarify these flaws and to indicate possible alternatives, the essence of the methodology is first outlined.

The logarithm of the transmissivity $Y(x,y) = \ln T(x,y)$ is viewed as a random field with Gaussian distribution. It is decomposed into its deterministic mean $F(x,y)$, also called the drift, and a random part $f(x,y)$, so that $Y = F + f$ with the expectation $E(f) = 0$. A stationary structure is assumed for the covariance Q_{ff} while the mean F is allowed to have a linear trend. A classical choice is

$$F = \mu_0 + \mu_1 x + \mu_2 y$$

$$Q_{ff}(z_1,z_2) = \theta_0 \delta(z_1,z_2) + \theta_1 \exp(-|z_1 - z_2|/\ell_f)$$

where $\{\mu_i\}$, $\{\theta_j\}$ and ℓ_f are the parameters to be determined, δ_{ij} is the Kronecker delta and $z \equiv (x,y)$.

For a given $Y = F + f$ the piezometric head is now decomposed into $\varphi = H + h$ where H and h are the deterministic and random components corresponding to F and f respectively. The boundary conditions and q are assumed to be fixed once and for all. In terms of logtransmissivity Y , equation (8) becomes

$$\nabla Y \cdot \nabla\varphi + \Delta\varphi = qe^{-Y} .$$

Replacing Y and φ by their respective values leads to

$$\nabla(F+f) \cdot \nabla(H+h) + \Delta(H+h) = qe^{-(F+f)} .$$

If it may be assumed that inner products of perturbation gradients are negligible, the equations for the mean and random terms are

(11) $$\nabla F \cdot \nabla H + \Delta H = qe^{-F}$$

(12) $$\nabla F \cdot \nabla h + \Delta h = -qe^{-F} f - \nabla H \cdot \nabla f .$$

Upon discretisation of the aquifer domain Ω , the mean piezometric head H is given by (11). At the discretisation nodes equation (12) now provides the matrix equation

(13) $$\mathbf{h} = \mathbf{K}\mathbf{f}$$

where $\mathbf{h}$ and $\mathbf{f}$ are vectors and K is a matrix that depends on the $\{\mu_i\}$. Exploitation of (13) provides a simple structure for the joint piezometric head and transmissivity random field at the measurement nodes with

$$E[\mathbf{h}] = KE[\mathbf{f}] = 0$$
$$Q_{hh} \equiv E[\mathbf{h}\mathbf{h}^T] = KE[\mathbf{f}\mathbf{f}^T]K^T \equiv KQ_{ff}K^T$$
$$Q_{hf} \equiv E[\mathbf{h}\mathbf{f}^T] = KE[\mathbf{f}\mathbf{f}^T] = KQ_{ff} .$$

The joint covariance matrix therefore becomes

$$Q = \begin{bmatrix} Q_{hh} & Q_{hf} \\ Q_{fh} & Q_{ff} \end{bmatrix} = \begin{bmatrix} KQ_{ff}K^T & KQ_{ff} \\ Q_{ff}K^T & Q_{ff} \end{bmatrix} . \tag{14}$$

At this stage the distinction must be drawn between measurement nodes and discretization nodes. On a 10km by 10km aquifer in which there are no large variations in transmissivity and piezometric head, a rectangular grid with 500m between points might be expected to give reasonable converge. This leads to a discretization relating head and transmissivity values at some 400 nodes. Actual head measurements are likely to be available at only some 50-100 nodes, and actual transmissivity measurements at only some 10 nodes (i.e. I~50, J~10). Therefore the vectors $\mathbf{h}$ and $\mathbf{f}$ must be split up into components $\begin{bmatrix} \mathbf{h}_k \\ \mathbf{h}_u \end{bmatrix}$ and $\begin{bmatrix} \mathbf{f}_k \\ \mathbf{f}_u \end{bmatrix}$ where $\mathbf{h}_k$, $\mathbf{f}_k$ are the known measurements $(\varphi_1,\ldots,\varphi_I)$ and $(Y_1,\ldots,Y_J)$ (minus the mean fields), and $\mathbf{h}_u$, $\mathbf{f}_u$ are the unknown values at the remaining nodes.

It remains to determine the parameters and unknown field components. In the geostatistical approach they are chosen so as to maximize the likelihood function, i.e. to solve

$$\max\ p(\mathbf{m}|\{\mu_i\},\{\theta_j\},\ell_f,\mathbf{h}_u,\mathbf{f}_u) \tag{15}$$
$$= \frac{1}{(2\pi)^N|Q|}\exp\left[-\frac{1}{2}(\mathbf{m}-E(\mathbf{m}))^T Q^{-1}(\mathbf{m}-E(\mathbf{m}))\right]$$

where $\mathbf{m}$ is the vector $\begin{bmatrix}\mathbf{h}\\ \mathbf{f}\end{bmatrix}$ and N is the size of the discretization.

In principle this minimization should be carried out simultaneously in all the unknowns. Since this is a nonlinear problem in several hundred variables in practice it is approximated by splitting it up into a series of smaller subproblems, such that each has a linear solution.

First the correlation length ℓ_f is specified in advance using prior knowledge (calculations have shown that the likelihood function is not very sensitive to changes in ℓ_f) . Next the parameters $\{\mu_i\}$ and $\{\theta_j\}$ are estimated by maximizing a reduced likelihood function. This is derived by eliminating the unknowns $\mathbf{h}_u$ and $\mathbf{f}_u$. Thus (13) is replaced by a coarser discretization

$$\mathbf{h}_K = \tilde{K}\mathbf{f}_K \tag{16}$$

that links only known data points, and $\mathbf{m}$ is replaced by $\mathbf{m}_K = \begin{bmatrix}\mathbf{h}_K\\ \mathbf{f}_K\end{bmatrix}$. This gives an approximate covariance structure for $\mathbf{h}$ and $\mathbf{f}$, and the unknowns $\mathbf{h}_u$ and $\mathbf{f}_u$ are now estimated by kriging.

However there are a number of drawbacks with the approach as outlined above. The first is that given the wide range of transmissivity values observed in practice it is by no means certain that the expansion in first order terms that leads to (11) and (12) is a sufficiently good approximation of the true system. This issue is further discussed in Appendix C.

The second drawback is more immediate. As Appendix B shows, the Q of (14) does not have an inverse, so the likelihood function of (15) is not well defined. This problem may be remedied in a number of ways. First, if (13) is kept as is, then (15) should be replaced by the constrained optimization problem:

$$\max\ p(\mathbf{f}\,|\,\{\mu_i\},\{\theta_j\},\ell_f,\mathbf{f}_u) \equiv \frac{1}{(2\pi)^{K/2}|Q_{ff}|}\exp\left[-\frac{1}{2}(\mathbf{f}-E(\mathbf{f}))^T Q_{ff}(\mathbf{f}-E(\mathbf{f}))\right]$$

subject to $\quad \mathbf{h}_K = [K\mathbf{f}]_K$.

However a more sensible approach is to note that (13) cannot be an exact relation as stated and that it should actually be written as

$$\mathbf{h} = K\mathbf{f} + \epsilon_M + \epsilon_D + \epsilon_T \tag{17}$$

where ϵ_M is the vector of errors made during actual head measurements, ϵ_D is the discretization error incurred in replacing the continuous fields by discrete pointwise approximations, and ϵ_T is the truncation error incurred by neglecting second order terms. It is reasonable to assume that these errors are uncorrelated with each other, have zero mean, and furthermore that if their covariance matrices are denoted by

R_M , R_D and R_T , that $R_M + R_D$ has a structure similar to Q_{ff} , i.e.

$$(R_M+R_D)(z_1,z_2) = \sigma_0\delta(z_1,z_2) + \sigma_1 \exp[-|z_1-z_2|/\ell_f] .$$

The structure of R_T is discussed in Appendix C .

If (13) is now replaced by (17) then

$$Q_{hh} = KQ_{ff}K^T + R_M + R_D + R_T$$

and if this is substituted into (14) then the overall covariance matrix Q is now invertible and the geostatistical approach may be carried out as described. However a further drawback is immediately apparent. If (13) is replaced by (16) the discretization error incurred will increase dramatically and is likely to be sufficiently great that (16) actually contributes very little towards estimation of Q_{ff} . Therefore the geostatistical approach as described will make no effective use of the flow equation.

Thus, if the information in the flow equation is to be used, the vector f_u must be chosen to be large enough to reduce the discretization error to within reasonable levels, and the likelihood function must be maximized simultaneously in both f_u and the parameters $\{\theta_j\}$ and $\{\sigma_k\}$. Unfortunately this is a large nonlinear problem; and the computational difficulty of solving it, together with the possible errors introduced by the approximations used in deriving the model leave the utility of the geostatistical approach open to question.

8. Conclusions

Motivation for solving inverse problems relating to the parameterisation of aquifer parameters has been provided. An analytical solution for the transmissivity T of a two-dimensional, confined and isotropic aquifer has been given and the structure of the solution illustrates the improperly posedness of this AI problem. Upon discretisation of the aquifer the interconnection between existence, uniqueness, stability and the level of parameterisation of the unknowns has been examined.

Tikhonov regularisation has been proposed as an obvious technique for stabilising the class of direct methods based on equation error criterion. The geostatistical approach to AI is analysed in some detail. Although its features are attractive it is demonstrated that linearisation of the perturbations equation is an over-simplification since it does not provide a covariance matrix that is positive definite. Recent work (Dietrich and Jakeman, 1986) questions the viability of this new method, given the strong assumptions needed to derive a solution.

Following discussion at the workshop, a new method based upon a weak formulation of the PDE (8) is being investigated (Dietrich and Anderssen, 1986). The formulation involves integrating both sides of the PDE against appropriate test functions so that the solution is found by variational methods. The main advantage of such an approach is that differentiation of the piezometric head φ may be transferred by integration by parts to differentiation of the test functions, which may

then be performed analytically. This overcomes the problem of instability due to the presence of high frequency noise in φ measurements. Initial results are encouraging for simulated two-dimensional aquifers where the basis functions $v_n(x,y)$ in (10) are exactly known and noise with normal distribution $N(0,\sigma^2)$ has been added to φ. Good estimates of the parameters τ_n in equation (10) have been obtained for value of σ^2 as high as ten per cent of the mean drop of the head over the domain Ω. However, the method appears to be sensitive to the choice of the basis function v_n. At the present stage, further work is required to improve and test the procedure so that comparisons can be made with other approaches to AI.

Appendix A

The governing PDE (8) with $\varphi(z)$ known and T being the dependent variable can be written as

(A1) $$\nabla T(z) \cdot \nabla\varphi(z) + T(z)\Delta\varphi(z) = q(z)$$

with Δ being the Laplace operator and $(z_1,z_2) \in \Omega$. Setting

$$\frac{\partial\varphi}{\partial z_i} = \frac{dz_i}{d\theta} \qquad i = 1,2$$

we obtain a family of characteristic curves $z(\theta)$ in Ω parameterised by θ. If Γ is one particular element of such a family, along Γ equation (A1) becomes

(A2) $$\frac{dT(z(\theta))}{d\theta} + T(z(\theta)) \Delta \varphi(z(\theta)) = q(z(\theta))$$

(A2) is a first order ordinary differential equation for $T(z(\theta))$ and its solution along the characteristic Γ is (Kaplan and Lewis, 1971)

$$T(z(\theta)) = \psi(\theta) \left[\int_0^\theta \frac{q(z(\eta))d\eta}{\psi(\eta)} + \text{const}\right]$$

with

$$\psi(\eta) = \exp\left[-\int_0^\eta \Delta\varphi(z(\xi))d\xi\right], \qquad \eta \in [0,\theta] .$$

Appendix B

If Q is a block matrix $\begin{bmatrix} A & B \\ C & D \end{bmatrix}$ with $|D| \neq 0$ we have (Graybill, 1983) $|Q| = |D|\ |A-BD^{-1}C|$.

Appendix C

An alternative approach that exploits the prior information represented by the PDE (8) and avoids making linear approximations is to assume a structure for Y and then derive a structure for φ via equations (11) and (12). In the case of a one-dimensional aquifer it is easy to show that if the transmissivity T is decomposed into its mean G and random component g, the corresponding random element h for the head φ satisfies the following matrix equation

(C1) $$\mathbf{h} = \sum_{i=1}^{\infty} K_i \, \boldsymbol{v}^{(i)}$$

where the vector $\boldsymbol{v} = \mathbf{g}/G$ is assumed to have norm < 1, $\boldsymbol{v}^{(i)}$ is the vector obtained from $\boldsymbol{v}$ by taking the i-th power of each component, and the K_i are matrices resulting from discretisation of (8).

If $\boldsymbol{v}$ is normally distributed then all odd moments are equal to zero, so that

$$E(\mathbf{h}) = \sum_{j=1}^{\infty} K_{2j} \, E[\boldsymbol{v}^{(2j)}] > 0 \ .$$

If only first and second order terms are taken in (14) we have

$$\mathbf{h} = K_1 \boldsymbol{v} + K_2 \boldsymbol{v}^{(2)}$$

so that

$$E[\mathbf{h}] = K_1 E[\boldsymbol{v}] + K_2 E[\boldsymbol{v}^{(2)}] = \sigma^2 \, K_2 \, \mathbf{e}$$

where $\mathbf{e}$ is a vector of unit elements and σ^2 is the variance of $\boldsymbol{v}$. The covariance matrix for the head Q_{hh} then becomes

$$Q_{hh} = E[\mathbf{h}\mathbf{h}^T] - E[\mathbf{h}]E[\mathbf{h}]^T$$

with

$$E[\mathbf{h}\mathbf{h}^T] = K_1 E[\boldsymbol{v}\boldsymbol{v}^T] \, K_1^T + K_1 E[\boldsymbol{v}\boldsymbol{v}^{(2)T}] K_2^T$$
$$+ K_2 E[\boldsymbol{v}^{(2)}\boldsymbol{v}^T] \, K_1^T + K_2 E[\boldsymbol{v}^{(2)}\boldsymbol{v}^{(2)T}] K_2^T$$

and

$$E[\mathbf{h}]E[\mathbf{h}]^T = \sigma^4 K_2 \mathbf{e}\mathbf{e}^T K_2^T \ .$$

Since all odd moments are equal to zero and the fourth moment $E[\boldsymbol{v}^{(2)}\boldsymbol{v}^{(2)T}]$ is equal to $\sigma^4 \mathbf{e}\mathbf{e}^T + 2\, Q_{vv}^{(2)}$ (Anderson, 1958) (where $Q_{vv}^{(2)}$ is obtained by multiplying each coefficient of Q_{vv} by itself), we obtain

$$Q_{hh} = K_1 Q_{vv} K_1^T + 2\, K_2\, Q_{vv}^{(2)}\, K_2^T$$

and

$$Q_{hv} = K_1 Q_{vv} \ .$$

The determinant of Q is now given by

$$|Q| = |Q_{vv}| \cdot |2\, K_2\, Q_{vv}^{(2)}\, K_2^T| \ .$$

Since Q_{vv} is assumed to be positive definite, $Q_{vv}^{(2)}$ is positive definite (Graybill, 1983) and, provided K_1 and K_2 are not singular, Q itself becomes positive definite.

Note that singularity may still result from ill-conditioning of K_1 or K_2. However, this would only reflect lack of independence in the available data.

Extension of equation (C1) to a two-dimensional aquifer is in general not possible since no explicit form for h as a function of the logtransmissivity perturbation f is available. For the particular case where the mean logtransmissivity is assumed constant, Dietrich and Jakeman (1986) use the Green's function for the two-dimensional Laplacian operator Δ to derive a formal expression for all terms involving first and second order perturbations. Since in most practical cases the Green's function is not known due to the complicated geometry of the aquifer boundary, simplifying assumptions have to be invoked. Dietrich and Jakeman (1986) show that if the aquifer is strongly excited by an inflow q assumed to be non zero everywhere, or if f and Δf remain small while q is set to zero, then second order perturbations can be derived without explicit knowledge of the Green's function. However, such assumptions are seldom valid. Therefore it is argued thus that these difficulties further limit the generality of the geostatistical approach to AI.

10. References

[1] Allison, H.J. and Peck, A.J. (1985). *Inverse problems for groundwater research.* Hydrology and Water Resources Symposium, Sydney, pp 20-24.

[2] Anderson, T.W. (1958). *An Introduction to Multivariate Statistical Analysis.* Wiley and Sons, p 39.

[3] Bakr, A.A., Gelhar, L.W., Gutjahr, A.L. and Macmillan, J.R. (1978). *Stochastic analysis of spatial variability in subsurface flows 1: Comparison of one and three-dimensional flows.* Water Resour. Res., Vol. 14, pp 263-271.

[4] Bastin, G. (1981). *Identification of steady-state distributed systems with space-variable parameters.* Proc. 6th IFAC World Congress, Kyoto, Japan. Vol. 2, pp 64-69.

[5] Bear, J. (1972). *Dynamics of Fluids in Porous Media.* New York, Elsevier.

[6] Bouwer, H. (1978). *Groundwater Hydrology*. New York, McGraw-Hill.

[7] Carrera, J. and Neuman, S.P. (1986). *Estimation of aquifer parameters under transient and steady state conditions 1: Maximum likelihood method incorporating prior information*. Water Resour. Res., Vol. 22, pp 199-210.

[8] Chavent, G. (1971). *Analyse fonctionnelle et identification de coefficients repartis dans les equations aus derivees partielles*. PhD thesis, Fac. of Sci., Univ. of Paris.

[9] Chavent, G., Dupuy, M. and Lemonnier, P. (1975). *History matching by use of optimal control theory*. Soc. Pet. Eng. J., Vol. 15, pp 74-86.

[10] Chen, W.H., Gavalas, G.R., Seinfeld, J.H. and Wasserman, M.L. (1974). *A new algorithm for automatic history matching*. Soc. Pet. Eng. J., Vol. 14, pp 593-608.

[11] Cooley, R.L. (1977). *A method of estimating parameters and assessing reliability for models of steady state ground flow 1: Theory and numerical properties*. Water Resour. Res., Vol. 13, pp 318-324.

[12] Cooley, R.L. (1982). *Incorporation of prior information on parameters into nonlinear regression groundwater flow models 1: Theory*. Water Resour. Res., Vol. 18, pp 965-976.

[13] Courant, R. and Hilbert, D. (1962). *Methods of Mathematical Physics, Vol. 2*. New York, Wiley and Sons.

[14] Dagan, G. (1985). *Stochastic modeling of groundwater flow by unconditional and conditional probabilities: The inverse problem*. Water Resour. Res., Vol. 21, pp 65-72.

[15] Dietrich, C.R. and Anderssen R.S. (1986). *Aquifer identification using a weak formulation*, Working paper, Centre for Resource and Environmental Studies, Australian National University, Canberra.

[16] Dietrich, C.R., Anderssen R.S. and Jakeman, A.J. (1986). *Solving the inverse groundwater flow problem*. Hydrology and Water Resources Symposium, Brisbane, November 25-27.

[17] Dietrich, C.R. and Jakeman, A.J. (1986), *Stochastic assumptions in aquifer parameter estimation*. Submitted to Water Resour. Res.

[18] Freeze, R.A. and Cherry, J.A. (1979). *Groundwater*. New Jersey, Prentice-Hall Inc.

[19] Ghassemi, F., Jakeman, A.J., Thomas, G.A. and Daamen, C. (1986). *Salinity management in the Mildura area and the use of mathematical models*. Hydrology and Water Resources Symposium, Brisbane, November 25-27.

[20] Graybill, F.A. (1983). *Matrices with Applications in Statistics*. 2nd edition, Wadsworth International Group.

[21] Hoeksema, R.J. and Kitanidis, P.K. (1984). *An application of the geostatistical approach to the inverse problem in two-dimensional groundwater modeling*. Water Resour. Res., Vol. 20, pp 1003-1020.

[22] Hoeksema, R.J. and Kitanidis, P.K. (1985). *Comparison of Gaussian conditional mean and kriging estimation in the geostatistical solution of the inverse problem*. Water Resour. Res., Vol. 21, pp 825-836.

[23] Kaplan, W. and Lewis, D.J. (1971). *Calculus and Linear Algebra*. New York, Wiley and Sons.

[24] Kuiper, J. (1986). *A comparison of several methods for the solution of the inverse problem in two-dimensional steady state groundwater flow modeling*. Water Resour. Res., Vol. 22, pp. 705-714.

[25] Kravaris, C. and Seinfeld, J.H. (1985). *Identification of parameters in distributed parameter systems by regularisation*. SIAM J. Control and Opt., Vol. 23, pp 217-241.

[26] Lukas, M.A. (1980). *Regularization*, in *The application and numerical solution of integral equations*. Anderssen, R.S., et al., eds. Netherlands, Sijthoff and Noordhoff.

[27] Matheron, G. (1973). *The intrinsic random functions and their applications*. Adv. Appl. Prob., Vol. 5, pp 439-468.

[28] Neuman, S.P. and Yakowitz, S. (1979). *A statistical approach to the inverse problem of aquifer hydrology 1: Theory*. Water Resour. Res., Vol. 15, pp 845-860.

[29] Neuman, S.P. (1980). *A statistical approach to the inverse problem of aquifer hydrology 3: Improved solution method and added perspective*. Water Resour. Res., Vol. 16, pp 331-346.

[30] Papoulis, A. (1964). *Probability, Random Variables and Stochastic Processes*. New York, John Wiley.

[31] Pinder, G. F. and Gray, W.G. (1977). *Finite Element Simulation in Surface and Subsurface Hydrology*. New York, Academic Press.

[32] Sun, N.Z. and Yeh, W.W.G. (1985). *Identification of parameter structure in groundwater inverse problem*. Water Resour. Res., Vol. 21, pp 869-883.

Centre for Resource and Environmental Studies
Australian National University
CANBERRA ACT 2601