A One-Dimensional Study of the Groundwater Inverse Problem Using Sensitivity Analysis

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ABSTRACT

In this work, an indirect inverse method utilizing sensitivity analysis is employed to help understand the reasons for model insensitivity. The results of the sensitivity analysis allow the modeler to delineate insensitive areas of the model where inverse procedures will be more subject to error. Sensitivity coefficients are defined and discussed. A differential equation is developed for the sensitivity coefficients that will generally be solved by numerical techniques. A relatively simple least squares inverse procedure is used on a hypothetical model to illustrate typical problems that can be enountered. In particular, the effect of data accuracy is considered. The low sensitivity areas of models are generally related to small values of $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$. The fact that considerable error in the transmissivity and storativity may occur in areas of low sensitivity should not be looked upon as a failing of the inverse procedure. It is simply a fact that not all areas of the model have been stressed equally. The main advantage of the present work is that areas of low sensitivity may be delineated.

INTRODUCTION

The groundwater inverse problem has received much attention in the literature for several years. The following references are representative of that work: Vermuri and Karplus (1969), Kleinecke (1971), Yeh and Tauxe (1971), Emsellem and de Marsily (1971), Lovell _et al._ (1972), Knowles _et al._ (1972), Neuman (1973), Frind and Pinder (1973), Distefano and Rath (1975), Neuman and de Marsily (1976), Chang and Yeh (1976), Haimes (1977), Dogru _et al._ (1977), Cooley (1977), Wilson _et al._ (1978), Cooley (1979), Tang and Pinder (1979), Neuman and Yakowitz (1979), Birtles and Morel (1979), Neuman _et al._ (1980), and Neuman (1980). Most of the recent work has been done for steady state groundwater systems and has been concerned with developing improved techniques and algorithms for the so-called indirect methods.

In this work an indirect method is also considered. However, rather than concentrating on developing improved techniques and algorithms, this work is more concerned with understanding the reasons for model insensitivity and with developing a formalism that will allow the modeler to diagnose insensitive areas of the model. This formalism is sensitivity analysis; and it can provide valuable information on the reliability of the model. First sensitivity coefficients are defined and discussed. Then, a differential equation is developed for the sensitivity coefficients that will generally be solved by numerical techniques. The sensitivity coefficients can be used in an inverse procedure to estimate the aquifer transmissivity and storativity. A relatively simple least squares inverse procedure is outlined in this work.

The low sensitivity areas of models are generally related to small values of $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$. This means that the sensitivity varies spatialy and temporally. Consequently, at early times after pumping stresses are applied, at late times near the steady state, and near no-flow boundaries, the inverse procedure may have difficulty obtaining the desired accuracy. As might be expected the accuracy of input data (head values) is more critical in areas of low sensitivity. However, practically speaking, it may be impossible to continually decrease the error in transmissivity and storativity by giving increasingly accurate head values. These considerations may be further complicatd by an inherent nonuniqueness of the model. For example, if the model is only sensitive to the ratio of transmissivity to storativity, the two parameters will interact and neither can be more accurate than the other.

The inverse results obtained for a hypothetical model are presented to illustrate typical problems encountered with inverse procedures. The results of sensitivity analysis are used to help understand the various sources of error that may occur. In particular, the effect of data accuracy is considered.

SENSITIVITY COEFFICIENTS

When a model is used to describe the hydraulic head distribution (h) in a groundwater system, it is assumed that the head depends uniquely upon the physical parameters input to the model.

$$h = h(x,t;T(x),S(x),Q(x,t)) \tag{1}$$

T, S, and Q are respectively transmissivity, storativity, and flux of water in or out of the system. It has been assumed that the transmissivity and storativity do not depend upon time (t). This assumption means that unconfined aquifers with or without delayed yield will not be explicitly considered. One-dimensional models that depend only on one spatial coordinate (x) have been chosen for two reasons. First, the discussion is simplified considerably. Second, only general properties of sensitivity coefficients and the inverse problem will be considered. The results from the one-dimensional models should be applicable to two-dimensional models as long as the results are applied parallel to streamlines. In this work Q(x,t) will be assumed to be known. Only the variation of the model response to changes in T(x) and S(x) will be considered.

The sensitivity coefficients can be easily defined if the transmissivity and storativity do not vary with space (Tomovic, 1962; Vemuri, et al., 1969; McCuen, 1973; McElwee and Yukler, 1978).

$$U_T(x,t) = \frac{\partial h(x,t;T,S,Q)}{\partial T} \tag{2a}$$

$$U_S(x,t) = \frac{\partial h(x,t;T,S,Q)}{\partial S} \tag{2b}$$

Therefore, the change in head (Δh) at any point due to a small change in transmissivity (ΔT) is given by

$$\Delta h(x,t;T,S,Q) = U_T(x,t)\ \Delta T \tag{3}$$

to first order in ΔT. U_T shall be called the sensitivity coefficient with respect to changes in transmissivity. U_T also depends upon T, S, and Q; however, these dependences have not been explicitly indicated in equations (2) and (3) for simplicity. Equations similar to (2) and (3) may be written for the sensitivity with respect to changes in storativity (U_S).

In the more general case where transmissivity and storativity vary with space, a slightly different procedure is used to define the sensitivity coefficients. h will be the hydraulic head resulting from a transmissivity distribution T(x). Let h* represent the hydraulic head that results when the transmissivity distribution is changed at one point (x_o) by a small amount $\Delta T(x_o)$.

$$\frac{\Delta h(x,t;x_o)}{\Delta T(x_o)} = [h^*(x,t;T(x) + \delta(x-x_o)\Delta T(x_o),\ S(x),Q(x,t) \tag{4}$$
$$-h(x,t;T(x),S(x),Q(x,t))]/\Delta T(x_o)$$

The symbol $\delta(x-x_o)$ represents the Dirac delta function (Lighthill, 1958). It is assumed that x is a unitless variable so that $\delta(x-x_o)$ is also unitless. The sensitivity with respect to variations in transmissivity is defined as

$$U_T(x,t;x_o) = \lim_{\Delta T(x_o)\to 0} \frac{\Delta h(x,t;x_o)}{\Delta T(x_o)} \tag{5}$$

This sensitivity coefficient tells how much the head will be changed at point x due to a change in transmissivity $\Delta T(x_o)$ at point x_o. Since $\Delta T(x_o)$ is assumed to be small, a first-order expansion may be employed to obtain

$$h^* \cong h + U_T(x,t;x_o)\Delta T(x_o) \tag{6}$$

If the transmissivity is changed at more than one point, then the change in head Δh must be found by integrating over the area where T(x) is changed

$$h^* - h = \Delta h(x,t) = \int_{x_1}^{x_2} U_T(x,t;x_o)\Delta T(x_o)dx_o \tag{7}$$

Outside the region bounded by x_1 and x_2, $\Delta T(x_o)$ is zero. In the special case when the transmissivity is to be changed by a constant amount ΔT everywhere, equation (7) becomes

$$h^* - h = \Delta h(x,t) = \Delta T \cdot U_T(x,t) \tag{8}$$

where

$$U_T(x,t) = \int_{x_1}^{x_2} U_T(x,t;x_o)dx_o. \tag{9}$$

In the preceding development, x and x_o are assumed to be appropriate dimensionless variables.

A similar development for the sensitivity with respect to storativity (U_S) yields

$$h^*-h = \Delta h(x,t) = \int_{x_1}^{x_2} U_S(x,t;x_o)\Delta S(x_o)dx_o \qquad (10)$$

and

$$h^*-h = \Delta h(x,t) = \Delta S \int_{x_1}^{x_2} U_S(x,t;x_o)dx_o$$

when ΔS is constant over the region of integration. As before,

$$U_S(x,t;x_o) = \lim_{\Delta S(x_o)\to 0} \frac{\Delta h(x,t;x_o)}{\Delta S(x_o)} \qquad (11)$$

where

$$\begin{aligned}\Delta h(x,t;x_o) = {} & h^*(x,t;T(x),S(x) + \delta(x-x_o)\Delta S(x_o),Q(x,t)) \\ & - h(x,t;T(x),S(x),Q(x,t))\end{aligned} \qquad (12)$$

The sensitivity coefficients U_T and U_S are seen to be the quantities needed to calculate the response of a model to perturbations in the spatial distribution of transmissivity and storage. Consequently, a discussion of some of the general properties of sensitivity coefficients is in order. In later sections, procedures for determining sensitivity coefficients will be illustrated.

GENERAL PROPERTIES OF SENSITIVITY COEFFICIENTS

The general form of the one-dimensional flow equation is

$$\frac{\partial}{\partial x}\left[\frac{T(x)}{T_{max}}\frac{\partial h}{\partial x}\right] = \left[\frac{S_{max}}{T_{max}}\right]\left[\frac{S(x)}{S_{max}}\right]\frac{\partial h}{\partial t} - \frac{Q(x)}{\ell T_{max}\Delta x} . \qquad (13)$$

T_{max} and S_{max} are the maximum values of the transmissivity and storativity, respectively. $Q/\ell\Delta x$ is the specified water flux per unit area of the model. ℓ is the transverse (perpendicular to x) length and Δx is the length in the x direction over which Q is evenly distributed. Q is the volume of water per unit time that is recharge or discharge of the model. It will be convenient to assume x has been normalized so that it varies from zero to one. In addition to equation (13), boundary conditions and an initial condition are needed for the head. Typical boundary conditions are

$$h = H \text{ at } x=0 \text{ or } 1 \qquad (14)$$

$$\frac{\partial h}{\partial x} = -\frac{Q(x)}{\ell T(x)} \text{ at } x=0 \text{ or } 1. \qquad (15)$$

Many times it will be convenient to take the initial head distribution to be flat.

$$h(x,0) = \text{constant} \qquad (16)$$

Equations (13) through (16) illustrate how the head, and consequently the sensitivity coefficients, depend upon the transmissivity and storativity. The head can be written symbolically as

$$h = h\left(x, \frac{T_{max}}{S_{max}} t; \frac{T(x)}{T_{max}}, \frac{S(x)}{S_{max}}, \frac{Q(x)}{T_{max}}\right) \qquad (17)$$

provided Q and the boundary conditions do not depend upon time. If Q and the boundary conditions do depend upon time then additional time dependence besides $\frac{T_{max}}{S_{max}} t$ may be introduced in the head solution. Equation (17) shows that h and U_T depend on the transmissivity in three distinct ways. First, the time dependence causes h and U_T to be dependent upon the reference transmissivity T_{max}. Second, the spatial variation of transmissivity, $\frac{T(x)}{T_{max}}$, also influences h and U_T. Third, specified fluxes cause h and U_T to be dependent on transmissivity (T_{max}). Similarly, equation (17) shows that h and U_S depend on the storativity in two distinct ways. The reference storativity, S_{max}, appears in the time dependence of h and consequently U_S. Secondly, the spatial variation of storativity, $\frac{S(x)}{S_{max}}$, also influences h and U_S.

Consider the three ways that h and U_T depend on the transmissivity. Notice that at steady state the dependence on $\frac{T_{max}}{S_{max}} t$ disappears. If the model is using a constant value for transmissivity, then the dependence on $\frac{T(x)}{T_{max}}$ also disappears. The final dependence is given by the flux conditions and is seen to disappear if all specified fluxes are zero. Although it is rather unusual, if all these conditions hold, U_T is zero, indicating the model is not sensitive to the transmissivity. An example of this will be shown later. If all specified fluxes in the model are zero that means only barrier or specified head boundaries are used.

The dependence of U_S on the storativity is more simple. At steady state there is no dependence of h on S(x) or S_{max}; thus, U_S is zero at steady state.

If the homogeneous case is considered ($T(x)=T_{max}=T$, $S(x)=S_{max}=S$), equation (17) becomes

$$h = h(x, \frac{T}{S} t), \tag{18}$$

when all fluxes (Q) are zero. Using the definitions of U_T and U_S from equation (2), it is not difficult to show that

$$U_T = - \frac{S}{T} U_S \tag{19}$$

In this case the two sensitivity coefficients are not independent throughout the period of simulation. This means that any value of S and T will give a good solution as long as their ratio T/S is correct. In this case the inverse problem is nonunique.

Even if one allows spatial variation in T and S in equation (17), the inverse problem is still nonunique since any S_{max} and T_{max} having the same ratio will give an equally good solution provided there are no specified fluxes in the model. Theoretically, a specified flux at one point will uniquely determine the transmissivity distribution and consequently the storativity distribution. In practice there are other complications that introduce error in the inverse process. Some of these complications will be discussed later. Some inverse procedures (Knowles, et al., 1972) solve for the fluxes, Q, in addition to the transmissivity and storativity. The foregoing discussion and equation (17) show that, when both Q and T are adjusted, an additional level of nonuniqueness is introduced since only the ratios of Q and T need to be held constant.

Some initial condition must be specified for the hydraulic head at the beginning of a model simulation; consequently, this determines the initial condition on the sensitivity coefficients. The sensitivity coefficients may or may not start out zero. One commonly used initial condition is a flat original head distribution. In this case the sensitivity coefficients (U_T and U_S) have an initial value of zero. Another commonly used initial condition is a steady state head distribution. (Additional fluxes, $Q(x)$, are imposed and future changes are predicted.) For a steady state initial condition U_S is zero but U_T will not in general be zero. The initial values of U_T may be found by solution of equations to be discussed later.

The sensitivity coefficients indicate how the hydraulic head changes when the aquifer parameters are adjusted; therefore, it is logical to use the sensitivity coefficients in developing an inverse process for groundwater modeling. The details of the inverse procedure will be discussed in later sections. When the sensitivity coefficients are zero or not independent, it is clear that the inverse process will not work. This result is inherent in the model and does not depend on the details of the inverse process. In this case, the model simply has not been stressed properly to determine the aquifer parameters. In actual practice, the inverse process may experience difficulty when the sensitivity coefficients are very small but not zero. In this case, the model is simply not very sensitive to changes in aquifer parameters. By calculating and examining the sensitivity coefficients, one may obtain an indication of the stability of the inverse process.

SIMPLE EXAMPLES OF SENSITIVITY COEFFICIENTS

Consider a steady state one-dimensional model with no interior fluxes. Equation (13) becomes

$$\frac{\partial}{\partial x}\left[T(x)\,\frac{\partial h}{\partial x}\right] = 0. \tag{20}$$

The first integration of equation (20) gives

$$T(x)\,\frac{\partial h}{\partial x} = C = \text{constant.} \tag{21}$$

For boundary conditions, assume

$$h = H \qquad \text{at } x = R \tag{22}$$

and

$$\frac{\partial h}{\partial x} = -\,\frac{Q/\ell}{T(0)} \qquad \text{at } x = 0. \tag{23}$$

Integration of equation (21) yields the final solution for the hydraulic head

$$h(x) = \frac{QR}{\ell}\int_{x/R}^{1}\frac{dx'}{T(Rx')} + H. \tag{24}$$

The normalized variable x' = x/R has been introduced. Equation (24) allows for an arbitrary distribution of the transmissivity.

Consider the case of constant transmissivity in equation (24). The solution is

$$h(x) = \frac{Q}{\ell T}(R-x) + H. \tag{25}$$

Using the definition from equation (2) yields

$$U_T(x) = \frac{\partial h(x)}{\partial T} = \frac{Q}{\ell T^2}(x-R) = -\frac{s}{T}, \tag{26}$$

where s is the drawdown with reference to the constant head boundary.

$$s = h(x) - H = \frac{Q}{\ell T}(R-x) \tag{27}$$

This form (26) of the sensitivity coefficient is rather common (see McElwee and Yukler, 1978) and merely says that the model is more sensitive to transmissivity in areas having larger drawdown. Notice that, as the constant head boundary is approached, the sensitivity coefficient (U_T) goes to zero. The sensitivity with respect to storativity, U_S, is zero since only the steady state is being considered.

The sensitivity coefficients for an arbitrary transmissivity distribution can be found by considering the head solution, equation (24), and the definition of the sensitivity coefficient, equation (5). The new head caused by changing the transmissivity at one point (x_o) is

$$h^*(x) = \frac{QR}{\ell}\int_{x/R}^{1} \frac{dx'}{T(Rx') + \delta(Rx'-x_o)\Delta T(x_o)} . \tag{28}$$

The sensitivity coefficient developed from (5) is as follows:

$$U_T(x;x_o) = \begin{cases} -\dfrac{QR}{\ell}\dfrac{1}{T^2(x_o)} & \text{if } x \leq x_o \leq R \\ 0 & \text{if } x_o < x \end{cases} \tag{29}$$

This sensitivity coefficient is inversely proportional to the square of the transmissivity. Thus, areas of low transmissivity have a larger affect on model results than areas of high transmissivity. Also, notice that the transmissivity for x values less than the observation point, x, do not affect model results at the observation point. The sensitivity coefficient resulting from changing the transmissivity a constant amount ΔT over the whole model area (equation 9) is obtained by integrating equation (29).

$$U_T(x) = \int_0^1 U_T(x;Rx_o')dx_o' = -\frac{QR}{\ell}\int_{x/R}^1 \frac{dx_o'}{T^2(Rx_o')} \tag{30}$$

The normalized integration variable $x_o' = x_o/R$ has been introduced. If the transmissivity is constant, equation (30) becomes identical with equation (26).

Typically, numerical methods are used to solve the model equations when the transmissivity is allowed to vary in an arbitrary manner. Assume a constant node spacing (Δx) grid system has been set up such that

$$N\Delta x = R,$$

where N+1 is the total number of nodes (x = 0 is the first node). The head at point x_i ($x_i = i\Delta x$) is obtained from equation (25) by the following replacement.

$$R \int_{x_i/R}^{1} dx' \rightarrow \Delta x \sum_{k=i}^{N}$$

Assuming that a constant transmissivity exists between points k and k+1 ($T_{k+1/2}$), equation (25) becomes

$$h_i = \frac{Q\Delta x}{\ell} \sum_{k=i}^{N} \frac{1}{T_{k+1/2}} + H \qquad (31)$$

The sensitivity coefficient is obtained by differentiating equation (31).

$$U_{T_{i;j}} = \frac{\partial h_i}{\partial T_{j+1/2}} = \begin{cases} -\dfrac{Q\Delta x}{\ell} \dfrac{1}{T^2_{j+1/2}} & \text{if } j > i \\ 0 & \text{otherwise} \end{cases} \qquad (32)$$

This result could have been obtained from equation (29) simply by integrating the effect of a constant transmissivity over one node spacing. Much of this paper will deal with numerical models and the notation introduced in equation (32) will be used throughout. The sensitivity coefficient $U_{Ti;j}$ represents the change in hydraulic head at node point i due to a change in the transmissivity at $j+1/2$

The last simple example of sensitivity coefficienits involves a steady state one-dimensional model with the head specified at both boundaries.

$$h = H_1 \text{ at } x = 0 \tag{33a}$$

$$h = H_2 \text{ at } x = R \tag{33b}$$

Equations (20) and (21) are still valid for this model. Integrating equation (21) yields

$$h(x) = C \int_{x/R}^{1} \frac{dx'}{T(Rx')} + H_2 , \tag{34}$$

where C is a constant to be determined from the boundary condition at x=0. Putting x=0 in equation (34) results in the following expression for C.

$$C = (H_1 - H_2) / \int_{0}^{1} \frac{dx'}{T(Rx')} \tag{35}$$

If T is constant, equations (34) and (35) yield

$$h(x) = \left(\frac{H_2 - H_1}{R}\right) x + H_1 \tag{36}$$

Since equation (36) does not depend on the transmissivity,

$$U_T(x) = \frac{\partial h(x)}{\partial T} = 0. \qquad (37)$$

When the transmissivity is not constant, the sensitivity coefficients can be obtained by applying the definition, equation (5):

$$U_T(x;x_o) = \left[h(x)-H_2 + (H_2-H_1)\,\Theta\,(x_o-x)\right] / \left[T^2(x_o) \int_0^1 \frac{dx'}{T(Rx')}\right] \qquad (38)$$

$\Theta(x_o-x)$ is the Heaviside unit step function.

$$\Theta(x_o-x) = \begin{cases} 1 & \text{if } x_o > x \\ 0 & \text{if } x_o < x \end{cases} \qquad (39)$$

$h(x)$ is given by equations (34) and (35). Equation (38) shows that $U_T(x;x_o)$ has both negative and positive areas. If it is assumed that $H_1>h(x)>H_2$, $U_T(x;x_o)$ is negative for $x_o>x$ and positive for $x_o<x$. The sensitivity coefficient resulting from a constant change in the transmissivity, ΔT, everywhere can be obtained by integrating equation (38).

$$U_T(x) = \left[(h(x)-H_2) \int_0^1 \frac{dx'_o}{T^2(Rx'_o)} + (H_2-H_1) \int_{x/R}^1 \frac{dx'_o}{T^2(Rx'_o)}\right] / \int_0^1 \frac{dx'}{T(Rx')} \qquad (40)$$

If T is constant $U_T(x)$ is zero, as was already known from equation (37). Thus, the model becomes less sensitive to the value of T as a constant value of T is approached.

The numerical solution for the above model with constant node spacing (Δx) may be obtained as before by replacing the integrals in equation (34) and (35) with the appropriate summations.

$$h_i = \frac{(H_1 - H_2)}{\sum\limits_{k=0}^{N} \frac{1}{T_{k+1/2}}} \sum_{k=i}^{N} \frac{1}{T_{k+1/2}} + H_2 \tag{41}$$

The sensitivity coefficient $U_{Ti;j}$ can be obtained from equation (41) by differentiation.

$$U_{Ti;j} = \frac{\partial h_i}{\partial T_{j+1/2}}$$

$$U_{Ti;j} = \left[h_i - H_2 + (H_2 - H_1)\Theta(j-i)\right] / \left[T^2_{j+1/2} \sum_{k=0}^{N} \frac{1}{T_{k+1/2}}\right] \tag{42}$$

This equation is the discrete equivalent of equation (38). $U_{Ti;j}$ represents the change in hydraulic head at node point i due to a change in transmissivity at $j+1/2$

These simple examples of sensitivity coefficients have been presented to illustrate calculational procedures and some of the general properties of sensitivity coefficients discussed earlier. In the more general case, closed-form expressions for the hydraulic head and the sensitivity coefficients cannot be obtained.

DIFFERENTIAL EQUATION FOR SENSITIVITY COEFFICIENTS

For the general time-dependent case when transmissivity and storativity can vary spatially, there is no closed-form expression for the head and the sensitivity coefficients. The head is given by the solution of the following partial differential equation.

$$\frac{\partial}{\partial x}\left[T(x)\,\frac{\partial h}{\partial x}\right] = S(x)\,\frac{\partial h}{\partial t} - \frac{Q(x)}{\ell \Delta x} \qquad (43)$$

A partial differential equation for the sensitivity with respect to transmissivity can be developed by applying some of the definitions given earlier. If h* is the new head that results when the transmissivity is changed by $\Delta T(x_o)$ at x_o, then

$$\frac{\partial}{\partial x}\left[T(x)\,\frac{\partial h^*}{\partial x}\right] + \frac{\partial}{\partial x}\left[\delta(x-x_o)\,\Delta T(x_o)\,\frac{\partial h^*}{\partial x}\right] = S(x)\,\frac{\partial h^*}{\partial t} - \frac{Q(x)}{\ell \Delta x}\,. \qquad (44)$$

Applying the definition of $U_T(x,t;x_o)$, equation (5) results in the following expression:

$$\frac{\partial}{\partial x}\left[T(x)\,\frac{\partial U_T(x,t;x_o)}{\partial x}\right] + \frac{\partial}{\partial x}\left[\delta(x-x_o)\,\frac{\partial h}{\partial x}\right] = S(x)\,\frac{\partial U_T(x,t;x_o)}{\partial t} \qquad (45)$$

In deriving equation (45), equation (43) has been subtracted from equation (44), the result divided by $\Delta T(x_o)$, and the limit taken as $\Delta T(x_o) \to 0$.

Equation (45) is a partial differential equation for $U_T(x,t;x_o)$ which looks very much like the original flow equation except for two differences. First, the fluxes (Q(x)) do not appear in equation (45). Second, there is an additional term involving the differentiation of a delta function.

Except in very simple cases, numerical methods must be used to solve equation (43). The question arises as to how equation (45) may be used with numerical methods to obtain $U_T(x,t;x_o)$. Only the term involving the differentiation of the delta function will be considered. The other terms in equation (45) are similar to terms in the flow equation (43) and may be handled similarly. The elementary central difference formula for the slope of an arbitrary function f(x) evaluated at point x_i is

$$\left[\frac{\partial f(x)}{\partial x}\right]_{x=x_i} \cong \frac{f_{i+1/2} - f_{i-1/2}}{\Delta x}, \tag{46}$$

where a uniformly spaced node system is assumed such that $x_i = i\Delta x$. Equation (46) must be applied twice to obtain the numerical equivalent of the delta function term in equation (45). The first application of (46) yields

$$\left[\delta(x-x_o)\,\frac{\partial h}{\partial x}\right]_{\substack{x=x_i\\ x_o=x_{j+1/2}}} = \frac{h_{i+1/2} - h_{i-1/2}}{\Delta x}\,\delta_{i,j+1/2}\;, \tag{47}$$

where $\delta_{i,j}$ is the Kronecker delta with the following properties:

$$\delta_{i,j} = \begin{cases} 1 \text{ if } i=j \\ 0 \text{ if } i\neq j \end{cases} \tag{48}$$

The second application of equation (46) yields

$$\frac{\partial}{\partial x}\left[\delta(x-x_o)\,\frac{\partial h}{\partial x}\right]_{\substack{x=x_i\\ x_o=x_{j+1/2}}} = \frac{(h_{i+1} - h_i)}{\Delta x^2}\,\delta_{i,j} - \frac{(h_i - h_{i-1})}{\Delta x^2}\,\delta_{i-1,j} \tag{49}$$

The transmissivity shall be specified midway between nodes; that is why x_o is evaluated at $j+1/2$

The partial differential equation for the sensitivity with respect to storativity is somewhat easier to obtain. If h* is the new head that results when the storativity is changed by $\Delta S(x_o)$ at x_o then

$$\frac{\partial}{\partial x}\left[T(x)\,\frac{\partial h^*}{\partial x}\right] = \left[S(x)+\delta(x-x_o)\Delta S(x_o)\right]\frac{\partial h^*}{\partial t} - \frac{Q(x)}{\ell \Delta x} \quad . \tag{50}$$

Subtracting equation (43) from equation (50), dividing by $\Delta S(x_o)$, and taking the limit as $\Delta S(x_o)\to 0$ results in the following equation

$$\frac{\partial}{\partial x}\left[T(x)\,\frac{\partial U_S(x,t;x_o)}{\partial x}\right] = S(x)\,\frac{\partial U_S(x,t;x_o)}{\partial t} + \delta(x-x_o)\,\frac{\partial h}{\partial t} \tag{51}$$

Recall that the definition of U_S is given by equation (11).

Once again equation (51) looks identical in form to the flow equation except there are no fluxes (Q(x)) and the delta function term has been added. The numerical solution of equation (51) is carried out in a manner similar to that used for the flow equation except for the delta function term. If equation (51) is to be evaluated at $x=x_i$, $x_o=x_{j+1/2}$ and $t=t^{n+1/2}$ (n^{th} time, not the power n), then

$$\left[\delta(x-x_o)\,\frac{\partial h}{\partial t}\right]_{\substack{x=x_i\\ x_o=x_{j+1/2}}}^{t=t^{n+1/2}} = \frac{h_i^{n+1} - h_i^n}{\Delta t}\,\delta_{i,j+1/2} \tag{52}$$

where Δt is the time step and h_i^n is the hydraulic head at node point i after n time steps.

If it is assumed that numerical methods have been used to obtain the solution to equation (43), the flow equation, then the h's appearing in equation (49) or (52) are known and pose no threat to a solution of equation

(45) or (51) for the sensitivity coefficients. The same numerical techniques used to solve the flow equation may be used to solve the sensitivity equations. In fact, the same computer code used for the flow equation can be used for the sensitivity equations by simply replacing the fluxes in equation (43) by the terms in equation (49) or (52). The system must be solved for each discrete value of x_o. A discussion of the application of numerical methods to the solution of the flow equation and the sensitivity equations can be found in the Appendix. Ultimately, a numerical solution for the following sensitivity coefficients must be obtained.

$$U^n_{Ti;j} = \frac{\partial h^n_i}{\partial T_{j+1/2}} \tag{53}$$

$$U^n_{Si;j} = \frac{\partial h^n_i}{\partial S_j} \tag{54}$$

The superscript n is used to denote the nth time step. The subscripts i and j are the usual node indices.

THE INVERSE PROBLEM

The inverse problem for groundwater modeling involves solving for the aquifer parameters (usually transmissivity and storativity) from known historical values of hydraulic head. Much work has been done on this problem through the years (refer to the references given in the introduction). The general conclusion is that the inverse process is nontrivial and fraught with difficulty and uncertainty. The aquifer parameters obtained from the inverse process may be nonunique, have large errors, or be completely unobtainable. The purpose of this section is to examine these problems systematically. Of course any modeling effort, and consequently any inverse process, is limited in accuracy by our knowledge of the basic hydrologic processes occurring and the mathematical equations chosen to represent them. These areas are beyond the scope of the present paper. Assuming the correct mathematical model has been formulated, this paper will examine the effects of insensitive areas of the model and inaccurate historical head data.

One of the simplest inverse problems can be examined by taking the solution to a steady state one-dimensional model and solving for the transmissivity. The steady state form of equation (43) is

$$\frac{\partial}{\partial h}\left[T(x)\,\frac{\partial h}{\partial x}\right] = -\,\frac{Q(x)}{\ell \Delta x}\ . \tag{55}$$

The first integration of this equation gives

$$T(x)\,\frac{\partial h}{\partial x} = -\,\frac{1}{\ell \Delta x}\int Q(x)dx + C \tag{56}$$

where C is a constant to be determined by the boundary conditions. Solving equation (56) for T(x) results in

$$T(x) = \left[- \frac{1}{\ell \Delta x} \int Q(x)dx + C\right] / \frac{\partial h}{\partial x} \quad (57)$$

Obviously this procedure is indeterminant for areas of the model where $\frac{\partial h}{\partial x} = 0$. However, the procedure can also have difficulty in areas where $\frac{\partial h}{\partial x}$ is small but not zero.

Following Neuman (1975), assume that the heads are known only within an accuracy of ε. The transmissivity from equation (57) is

$$T^*(x) = \left[- \frac{1}{\ell \Delta x} \int Q(x)dx + C\right] / \left[\frac{\partial (h+\varepsilon)}{\partial x}\right] \quad (58)$$

The error in transmissivity is given by subtracting equation (57) from (58)

$$|T-T^*| = \left|- \frac{1}{\ell \Delta x} \int Q(x)dx + C\right| \left|\frac{\partial \varepsilon}{\partial x}\right| / \left|\frac{\partial h}{\partial x}\left(\frac{\partial h}{\partial x} + \frac{\partial \varepsilon}{\partial x}\right)\right| \quad (59)$$

Neuman argues that although the error in head may be bounded, that does not restrict $\frac{\partial \varepsilon}{\partial x}$. Consequently he blames $\frac{\partial \varepsilon}{\partial x}$ for the large variations in transmissivity that may occur. However, in the typical numerical model, $\frac{\partial \varepsilon}{\partial x}$ would be approximated by $\frac{\Delta \varepsilon}{\Delta x}$. If ε_{MAX} is the largest error in the head anywhere in the model area then

$$\frac{\partial \varepsilon}{\partial x} \cong \frac{\Delta \varepsilon}{\Delta x} \leq \frac{2\varepsilon_{MAX}}{\Delta x} . \quad (60)$$

Typically Δx is at least several hundred feet and ε_{MAX} is of the order of a few feet. Therefore, $\frac{\partial \varepsilon}{\partial x}$ is a small number for most typical models and it is difficult to see how that would cause large values of $|T-T^*|$.

Manipulating equation (59) slightly yields

$$\left|\frac{T-T^*}{T}\right| = \left|\frac{\partial \varepsilon}{\partial x}\right| / \left|\frac{\partial h}{\partial x} + \frac{\partial \varepsilon}{\partial x}\right| \tag{61}$$

Equation (61) shows that, in areas where $\frac{\partial h}{\partial x}$ and $\frac{\partial \varepsilon}{\partial x}$ are of the same order of magnitude and have differing signs, large errors in transmissivity may occur since it is possible for the denominator to approach zero. The conclusion to be drawn from equation (61) is that the effect of error in the head is much more pronounced in areas having a small hydraulic gradient that can be badly misrepresented. From this analysis, it is seen that an accurate representation of a nonzero hydraulic gradient is the prerequisite to a stable direct inverse procedure.

A numerical direct inverse procedure for the steady state can be implemented by use of numerical methods on equation (43).

$$-T_{i-\frac{1}{2}}(h_i-h_{i-1}) + T_{i+\frac{1}{2}}(h_{i+1}-h_i) = -\frac{Q_i\Delta x}{\ell} \tag{62}$$

Suppose that, at $x=\Delta x/2$, $Q_{\frac{1}{2}}/\ell$ is the specified flux per unit transverse width of the model; and at $x=R$ the head is specified to be H. These boundary conditions in equation form are

$$\frac{h_1-h_o}{\Delta x} = -Q_{\frac{1}{2}}/(\ell T_{\frac{1}{2}}) \tag{63}$$

and

$$h_{N+1} = H \tag{64}$$

Equation (63) is given by a simple application of Darcy's Law. Assuming that the heads and Q's are known, a system of equations can be written for the T's.

$$\begin{bmatrix} (h_2-h_1) & 0 & 0 & \cdots & 0 & 0 \\ -(h_2-h_1) & (h_3-h_2) & 0 & \cdots & 0 & 0 \\ 0 & -(h_3-h_2) & (h_4-h_3) & \cdots & 0 & 0 \\ \cdot & & & & \cdot & \cdot \\ \cdot & & & & \cdot & \cdot \\ \cdot & & & & \cdot & \cdot \\ 0 & 0 & \cdots & & -(h_N-h_{N-1}) & (H-h_N) \end{bmatrix} \begin{bmatrix} T_{3/2} \\ T_{5/2} \\ T_{7/2} \\ \cdot \\ \cdot \\ \cdot \\ T_{N+1/2} \end{bmatrix} = -\frac{\Delta x}{\ell} \begin{bmatrix} Q_{1/2}+Q_1 \\ Q_2 \\ Q_3 \\ \cdot \\ \cdot \\ \cdot \\ Q_N \end{bmatrix} \tag{65}$$

Notice that $T_{1/2}$ does not appear in the system of N equations; hence, it cannot be determined. If this system of equations is to have a solution, the determinant of the coefficient matrix must not be zero.

$$(h_2-h_1)(h_3-h_2)(h_4-h_3) \cdots (h_N-h_{N-1})(H-h_N) \neq 0 \tag{66}$$

Thus if the hydraulic gradient between node points is zero anywhere, a solution does not exist. Logically, in areas of small hydraulic gradient the model is less sensitive and the inverse procedure may have trouble computing correct values of the transmissivity. As pointed out earlier, errors in the hydraulic head may exaggerate this difficulty.

Changing the boundary conditions assumed for equation (65) does not change the above conclusions. However, if the flow had been specified at both ends of the model, there would be only N-1 independent values of transmissivity to be found from N-1 equations instead of the N equations contained in (65). If the head had been specified on both ends of the model then $T_{1/2}$ would have appeared as an additional unknown in (65). This would give N+1 unknowns and only N equations. The transmissivity must be known at one node point for there to be a unique solution of this system of equations. This need to know the transmissivity along a streamline has been pointed out by Emsellem and de Marsily (1971).

Most modeling projects involve time dependent flow. Consequently, an inverse procedure to find both T and S is most desirable. Using the numerical analog of equation (43) along with the boundary conditions given by equations (63) and (64), the following system of N equations can be written.

$$
\begin{aligned}
(h_2^{n+1/2}-h_1^{n+1/2})T_{3/2}-(h_1^{n+1}-h_1^{n})\,\frac{(\Delta x)^2}{\Delta t}\,S_1 &= -\frac{(Q_{1/2}+Q_1)\Delta x}{\ell}\\
-(h_2^{n+1/2}-h_1^{n+1/2})T_{3/2}+(h_3^{n+1/2}-h_2^{n+1/2})T_{5/2}-(h_2^{n+1}-h_2^{n})\frac{\Delta x^2}{\Delta t}S_2 &= -\frac{Q_2\Delta x}{\ell}\\
\cdot \qquad\qquad\qquad\qquad \cdot \qquad & \qquad \cdot\\
\cdot \qquad\qquad\qquad\qquad \cdot \qquad & \qquad \cdot\\
\cdot \qquad\qquad\qquad\qquad \cdot \qquad & \qquad \cdot\\
-(h_N^{n+1/2}-h_{N-1}^{n+1/2})T_{N-1/2}+(H-h_N^{n+1/2})T_{N+1/2}-(h_N^{n+1}-h_N^{n})\frac{\Delta x^2}{\Delta t}\,S_N &= -\frac{Q_N\Delta x}{\ell} \qquad (67)
\end{aligned}
$$

There are 2N unknowns (N values of transmissivity and N values of storativity) and only N equations in this system. Consequently the equations contained in (67) must be written at two different time levels in order to obtain 2N equations. As always for a solution to exist, the determinant of the coefficient matrix must not be zero.

The unknowns shall be arranged in the following order.

$$(T_{3/2}, T_{5/2}, \cdots, T_{N+1/2}, S_1, S_2, \cdots, S_N)$$

The necessary condition for solution, that the determinant of the coefficient matrix not be zero, leads to the following relation.

$$(-1)^N \frac{(\Delta x)^{2N}}{(\Delta t)^N} [(h_2^{n+1/2} - h_1^{n+1/2})(h_3^{n+1/2} - h_2^{n+1/2}) \cdots (H - h_N^{n+1/2})(h_1^{n+2} - h_1^{n+1})(h_2^{n+2} - h_2^{n+1}) \cdots$$
$$(h_N^{n+2} - h_N^{n+1}) + (h_2^{n+3/2} - h_1^{n+3/2})(h_3^{n+3/2} - h_2^{n+3/2}) \cdots (H - h_N^{n+3/2})(h_1^{n+1} - h_1^n)$$
$$(h_2^{n+1} - h_2^n) \cdots (h_N^{n+1} - h_N^n)] \neq 0 \qquad (68)$$

This relation shows that if any hydraulic gradient is zero over these two time intervals the determinant is zero and the system of equations has no solution. Similarly, if the head does not change with time at every node point for these two time intervals then the system again has no solution.

It is clear that the important quantities are $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$; they cannot be zero for significant time periods if the direct inverse process is to succeed. In regions where these quantities are small, the model is not very sensitive to the aquifer parameters and the direct inverse process may have difficulty. As discussed earlier, error in the head values (ε) will be more critical in regions where $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$ are small. This is because $\frac{\partial \varepsilon}{\partial x}$ and $\frac{\partial \varepsilon}{\partial t}$ may be of the same order of magnitude as $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$. Although these results have been obtained from equation (43) using the Crank-Nicolson differencing scheme, it can be shown that the results are independent of the differencing scheme (i.e., implicit or explicit could also be used).

As in the steady state case, changing the boundary conditions has no significant effect on the stated results. If the flow had been specified at both ends $T_{N+1/2}$ would not appear in the system of equations. This would leave 2N equations for 2N-1 unknowns (N-1 values of transmissivity and N values of storativity). If the head had been specified at both ends, $T_{1/2}$ would have appeared in (67) resulting in 2N+1 unknowns and only 2N equations, if only two time intervals are used. In this case one value of transmissivity must be known for a unique solution. (Alternately, an additional time step could be considered.)

LEAST SQUARES INVERSE PROCEDURE

In the previous section the so-called "direct" inverse process was discussed. In that procedure the number of unknown aquifer parameters and the number of equations are the same. Any of the common solution techniques for systems of equations could be used to obtain a direct solution. As pointed out in the previous section only two time intervals are needed to solve for all the aquifer parameters. (In some cases the transmissivity must be known at one node point.) In general, historical head data for the area to be modeled may be available for any number of previous times. Ideally one would like to use all these data to obtain the best estimate of transmissivity and storativity. If data are available over more than two time intervals, it is clear that the system is overdetermined and that parameters calculated directly over various time intervals may not agree due to error in the head values. The so-called "indirect" inverse procedures attempt to calculate the "best" transmissivity and storativity by minimizing some error functional. In this case the aquifer parameters obtained do not exactly satisfy the direct equations over any time interval. Rather, the best average solution is obtained over the historical period of record.

The objective of this section is to use the sensitivity coefficients in an indirect inverse procedure in such a way as to avoid some of the problems associated with direct inverse procedures. Suppose that initial estimates for T and S can be made, and that h_i^n is the head calculated from the model at node point i and time step n. If all the aquifer parameters are changed by some amount (ΔT_j or ΔS_j), the new head h_i^{*n} is given by

$$h_i^{*n} = h_i^n + \sum_j (U_{Ti;j}^n \Delta T_j + U_{Si;j}^n \Delta S_j). \qquad (69)$$

This equation is the numerical equivalent of the sum of equations (7) and (10). If he_i^n is the experimentally measured head at node point i for time step n, it would be desirable to choose ΔT_j and ΔS_j in such a way as to minimize the difference between h* and he. The error functional chosen to be minimized is the sum of the squared errors over all node points and time steps.

$$
\begin{aligned}
E(\Delta T_j, \Delta S_j) &= \sum_n \sum_i \; [he_i^n - h_i^{*n}]^2 \\
&= \sum_n \sum_i \; [(he_i^n - h_i^n)^2 - 2(he_i^n - h_i^n)\sum_j (U_{Ti;j}^n \Delta T_j + U_{Si;j}^n \Delta S_j) \\
&\qquad + (\sum_j U_{Ti;j}^n \Delta T_j + \sum_j U_{Si;j}^n \Delta S_j)^2] \qquad (70)
\end{aligned}
$$

A necessary condition for minimization of $E(\Delta T_j, \Delta S_j)$ is that the partial derivatives with respect to ΔT_j or ΔS_j be zero. Consider the derivative with respect to ΔT_j first.

$$
\begin{aligned}
\frac{\partial E(\Delta T_j, \Delta S_j)}{\partial \Delta T_j} = \sum_n \sum_i \; [-2(he_i^n - h_i^n) U_{Ti;j}^n + 2\sum_k (U_{Ti;k}^n \Delta T_k + U_{Si;k}^n \Delta S_k) \\
\cdot U_{Ti;j}^n] = 0 \qquad (71)
\end{aligned}
$$

By defining the quantities

$$
\alpha_{j,k} = \sum_n \sum_i \; U_{Ti;j}^n \, U_{Ti;k}^n \qquad (72)
$$

$$
\beta_{j,k} = \sum_n \sum_i \; U_{Ti;j}^n \, U_{Si;k}^n \qquad (73)
$$

$$f_j = \sum_n \sum_i U^n_{Ti;j}(he^n_i - h^n_i) \tag{74}$$

equation (71) may be written

$$\sum_k \alpha_{j,k}\Delta T_k + \sum_k \beta_{j,k}\Delta S_k = f_j. \tag{75}$$

Equation (75) may be written for each of the assumed N values of j. Similarly, the partial derivative of (70) with respect to ΔS_j may be taken and set equal to zero.

$$\frac{\partial E(\Delta T_j,\Delta S_j)}{\partial \Delta S_j} = \sum_n \sum_i \left[-2(he^n_i - h^n_i)U^n_{Si;j} + 2\sum_k (U^n_{Ti;k}\Delta T_k + U^n_{Si;k}\Delta S_k) \cdot U^n_{Si;j}\right] = 0 \tag{76}$$

If two new quantities

$$\gamma_{j,k} = \sum_n \sum_i U^n_{Si;j}U^n_{Si;k} \tag{77}$$

$$g_j = \sum_n \sum_i U^n_{Si;j}(he^n_i - h^n_i) \tag{78}$$

are defined, equation (76) takes the form

$$\sum_k \beta_{k,j}\Delta T_k + \sum_k \gamma_{j,k}\Delta S_k = g_j. \tag{79}$$

Again, equation (79) may be written for the N values of j. Taken together, equations (75) and (79) form a set of 2N equations containing 2N unknowns (ΔT_j and ΔS_j).

Equations (75) and (79) may be written in matrix notation by making the following identifications.

$$\overline{\overline{\alpha}} = [\alpha_{j,k}] \tag{80}$$

$$\overline{\overline{\beta}} = [\beta_{j,k}] \tag{81}$$

$$\overline{\overline{\gamma}} = [\gamma_{j,k}] \tag{82}$$

$$\overline{\Delta T} = [\Delta T_j] \tag{83}$$

$$\overline{\Delta S} = [\Delta S_j] \tag{84}$$

$$\overline{f} = [f_j] \tag{85}$$

$$\overline{g} = [g_j] \tag{86}$$

$\overline{\overline{\alpha}}$, $\overline{\overline{\beta}}$, and $\overline{\overline{\gamma}}$ are NxN matrices while $\overline{\Delta T}$, $\overline{\Delta S}$, $\overline{f}$, and $\overline{g}$ are N element column vectors. Equations (75) and (79) become

$$\overline{\overline{\alpha}}\cdot\overline{\Delta T} + \overline{\overline{\beta}}\cdot\overline{\Delta S} = \overline{f} \tag{75'}$$

$$\overline{\overline{\beta}}^{+}\cdot\overline{\Delta T} + \overline{\overline{\gamma}}\cdot\overline{\Delta S} = \overline{g} \quad , \tag{79'}$$

where $\overline{\overline{\beta}}^{+}$ is the transpose of $\overline{\overline{\beta}}$. In the form of a single matrix equation

$$\begin{bmatrix} \bar{\bar{\alpha}} & \bar{\bar{\beta}} \\ \bar{\bar{\beta}} & \bar{\bar{\gamma}} \end{bmatrix} \begin{bmatrix} \overline{\Delta T} \\ \overline{\Delta S} \end{bmatrix} = \begin{bmatrix} \bar{f} \\ \bar{g} \end{bmatrix}. \tag{87}$$

Any standard matrix routine may now be used to solve for the ΔT_j and ΔS_j which will minimize the error functional.

Unless the initial estimates for transmissivity and storage are within about 20% of their correct values (McElwee and Yukler, 1978), the new aquifer parameters calculated from

$$T_j^{(m+1)} = T_j^{(m)} + \Delta T_j^{(m)} \tag{88}$$

and

$$S_j^{(m+1)} = S_j^{(m)} + \Delta S_j^{(m)} \tag{89}$$

the first time may not be good enough. The superscripts in parentheses represent iteration indices. Once a new set of aquifer parameters is calculated from equations (88) and (89), the new heads and sensitivity coefficients may be calculated and placed in equation (87) allowing the next iteration values of ΔT_j and ΔS_j to be found. This procedure may be continued until all ΔT_j and ΔS_j are smaller than some predetermined criteria. The procedure has good convergence properties; but, if the initial estimates are bad, the procedure may not converge well. This situation may be helped considerably by imposing a few physically based restrictions. For example, no T_j or S_j can be negative; and S_j must be less than or equal to one. Since this is a first order theory, equation (69) neglects terms of the order of $(\Delta T_j)^2$ or $(\Delta S_j)^2$ or higher. This is why it may take several iterations to converge satisfactorily. It has also been helpful to restrict the magnitude that ΔT_j or ΔS_j may have for any one iteration. The net result of this restriction on ΔT_j and ΔS_j is that the procedure may take more iterations to converge in some situations, but will converge for poorer initial estimates of transmissivity and storativity.

This inverse procedure has some advantages over the direct procedures. The sensitivity coefficients are a direct measure of the model sensitivity to parameter variations at various nodes. However, for a good sized model there are many sensitivity coefficients making it difficult to look at all of them. A good compromise is to look at the diagonal elements of the coefficient matrix in equation (87). There are two types of diagonal elements.

$$\alpha_{jj} = \sum_n \sum_i U^n_{Ti;j} U^n_{Ti;j} \tag{90}$$

$$\gamma_{jj} = \sum_n \sum_i U^n_{Si;j} U^n_{Si;j} \tag{91}$$

The α_{jj} give a good indication of the total model sensitivity to the transmissivity at node j. Similarly, the γ_{jj} are indicators of the total model sensitivity to the storativity at node j. Examining these diagonal elements will quickly show the relative sensitivity of various areas of the model. Obviously, in areas of low sensitivity the calculated transmissivity or storativity distribution is more in doubt than in areas of high sensitivity. These areas of low sensitivity are where the direct method would have trouble and where errors in the experimental head will be most troublesome. In the extreme limit that one diagonal element is exactly zero, the direct method becomes indeterminant and ΔT_j or $\Delta S_j = 0$ is appropriate for the present procedure. This means that the initial estimate would not be changed at all. The fact that considerable error in S and T may result in areas of low or zero sensitivity should not be looked upon as a failing of the inverse procedure. It is simply a fact that not all areas of the model have been stressed equally. Until additional experimental head data become available to establish a minimum sensitivity level in all areas of the model, it is not possible to accurately estimate the transmissivity and storativity everywhere. The main advantage of the present procedure is that the areas of low sensitivity can be delineated.

HYPOTHETICAL MODEL

Figure 1 shows a hypothetical one-dimensional model chosen to illustrate the use of sensitivity coefficients in the inverse procedure. The model has a constant head boundary on the right and a barrier boundary on the left. The model is discretized by using a node spacing of 1,000 feet. The barrier boundary is located halfway between nodes 0 and 1. Node 0 is a fictitious point introduced to allow a second order correct approximation to $\frac{\partial h}{\partial x}$ (von Rosenberg, 1969). The constant head boundary is located at node 11. Therefore, it is 10,500 feet between boundaries. Nodes 0 and 11 can be eliminated from consideration by standard finite difference techniques. Thus, there are 10 equations (nodes 1 to 10) to be solved for the 10 unknown head values as a function of time.

The transmissivity and storativity are assumed to increase linearly from the barrier boundary to the constant head boundary. This is geologically reasonable and is consistent with the basic finite difference assumption that all spatially varying quantities can be linearly interpolated between node points. The transmissivity shall be specified midway between node points (for example, $T_{3/2}$ occurs between nodes 1 and 2). $T_{1/2}$ does not appear in the equations as long as the flux is specified at the left boundary; therefore, $T_{1/2}$ cannot be found by the inverse procedure. This leaves 10 values of transmissivity to be determined ($T_{1+1/2}$, $T_{2+1/2}$, ..., $T_{10+1/2}$). The storativity shall be specified at the node points. Only nodes 1 through 10 appear in the discretized flow equations, which means there are 10 values of storativity needed to describe this model. The assumed correct values for transmissivity and storativity are shown in Figure 1. $T_{3/2}$ is 52,000 gpd/ft (6952 ft^2/day) and the transmissivity increases by 2,000 gpd/ft (267 ft^2/day) as the node number increases by one. Thus, $T_{10+1/2}$ is 70,000 gpd/ft (9358

ft^2/day). The storativity at node 1 (S_1) is .0050 and increases by .0005 as the node number increases by one. Thus, S_{10} is .0095.

The initial head distribution is assumed to be flat. The aquifer is being pumped at a rate of Q equal to 1,500 gal/day (201 ft^3/day) per unit transverse length. The pumping occurs at node 7 and is 4,000 feet away from the constant head boundary. The model has a steady state solution where all water being pumped comes from the constant head boundary, and the head distribution to the left of the well is flat and somewhat lower than the original level.

This model was chosen because it illustrates some of the common features of models and because it illustrates some of the problems associated with the inverse solution. These typical problems will be pointed out in later sections.

INVERSE CALCULATIONS OVER VARIOUS TIME PERIODS

The correct values for the transmissivity at the 10 intermediate node points and for the storativity at the 10 node points are shown in the second column of Table 1. These values along with the other model parameters discussed in the previous section were used to generate hypothetical "field" data for the hydraulic head as a function of time. These values of hydraulic head were then used in the inverse procedure detailed earlier along with initial estimates for T and S in order to calculate the spatial variation of T and S. The initial estimate for transmissivity was 61,000 gpd/ft (8155 ft^2/day) and for storativity was .00725.

The transmissivity and storativity values calculated for early time by the inverse procedure are shown in the third column of Table 1. The early time calculations were made using hydraulic heads for 10 time steps with the total time slightly less than 2 days. For these early times the drawdown is less than 19 feet at the well and is less than one foot farther than three node points away from the well. The values of calculated transmissivity and storativity are within 20% of the actual values, but there is no clear evidence that the inverse procedure has been successful in finding the spatial trend of increasing T and S. At early time periods the drawdown is small and the model is fairly insensitive to the transmissivity and storativity. This insensitivity can be seen very easily by having the sensivitity coefficients (or the diagonal elements α_{jj} and γ_{jj}) printed out.

At middle times (column 4 of Table 1), when the drawdown is substantial and hydraulic heads are changing fairly rapidly with time, the greatest sensitivity and best inverse solution results. The middle time inverse calculations were made using hydraulic heads for 10 time steps between 2 days and 112 days. The system rapidly approaches steady state for times greater

TABLE 1. Inverse calculations over various time periods.

Grid Number	Correct Value	Early Time	Middle Time	Late Time
TRANSMISSIVITY (gpd/ft)				
1+½	52,000	59,575	48,415	72,213
2+½	54,000	62,107	55,064	69,827
3+½	56,000	64,365	55,980	71,049
4+½	58,000	66,684	57,955	70,520
5+½	60,000	69,070	60,000	71,130
6+½	62,000	71,283	62,002	243,374
7+½	64,000	55,152	64,001	64,006
8+½	66,000	56,931	66,000	65,998
9+½	68,000	58,603	68,000	67,998
10+½	70,000	60,330	70,000	69,998
STORATIVITY				
1	.0050	.0057	.004656	Unstable
2	.0055	.0063	.006037	Unstable
3	.0060	.0069	.005801	Unstable
4	.0065	.0075	.006491	Unstable
5	.0070	.0081	.007015	Unstable
6	.0075	.0086	.007501	Unstable
7	.0080	.0080	.007998	Unstable
8	.0085	.0073	.008501	Unstable
9	.0090	.0078	.009000	Unstable
10	.0095	.008	.009500	Unstable

than 112 days. The largest error in transmissivity is less than 7% and most values are very close to the correct values. The storativity calculations have less than 10% error and most are very close to the correct values. The largest errors occur near node 1. The reason for this will be discussed later.

The last column in Table 1 shows the transmissivity calculations as the model approaches steady state. The storativity calculations have become unstable and cannot be made because of low sensitivity. The late time inverse calculations have been made using hydraulic heads from 5 time steps between 112 days and 850 days. The transmissivity calculations for the last four node points are very good. However, the calculated transmissivities for the first six node points are fairly bad. This can be explained by looking at the sensitivity coefficients (or the diagonal elements α_{jj}). The sensitivity at the last four nodes is about three or four orders of magnitude greater than for the first six nodes. This lack of sensitivity is because $\frac{\partial h}{\partial x}$ is practically zero for the first six node points for times greater than 112 days.

MODEL SENSITIVITY TO TRANSMISSIVITY AND STORATIVITY

Notice that for the middle time calculations shown in Table 1, the largest error in transmissivity occurs at node one and decreases considerably at higher numbered nodes. This should mean that the model is least sensitive to T at node one. A look at the sensitivity coefficients should verify this. However, for a good sized model there are many sensitivity coefficients and it is difficult to look at all of them. For this model there are 100 sensitivity coefficients ($U_{Ti;j}$) for each time step. A good compromise is to look at the diagaonal elements of the system of equations to be solved for the ΔT's and ΔS's. These are shown as α_{jj} and γ_{jj} in Figure 2. The α_{jj} give a good indication of the total model sensitivity to the transmissivity at $j+\frac{1}{2}$. Notice that indeed the lowest sensitivity (α_{jj}) occurs at node one and is about three orders of magnitude smaller than the sensitivity for the last four nodes.

Table 1 shows that the largest errors in storativity also occur at the low numbered nodes for the middle time calculations. However, the plot of sensitivity for storativity (γ_{jj}) in Figure 2 shows that the least sensitive node is 10, while nodes 1 through 7 have roughly equal sensitivity. The explanation for this apparent contradiction is that T and S are not independent quantities near node 1. As discussed earlier (equation 19), the sensitivity coefficients may be related near a no flow boundary such as between nodes 0 and 1. This means that any ratio S/T with the correct value would work well there. From Table 1 it can be seen that .0050/52000 = .004656/48415. Thus, there is a basic nonuniqueness near node 1. α_{jj} is very low and causes error in the calculated T at node 1; this means that S will also be in error at node 1 such that S/T has the correct value even if γ_{jj} is reasonably large at node 1.

Examining the diagonal elements α_{jj} and γ_{jj} will quickly show the relative sensitivity of various areas of the model. The areas of low sensitivity show where the inverse process may have trouble and where errors in the hydraulic head measurements will be most troublesome. If some areas show extremely low sensitivity, it may be necessary to drop those areas from consideration in the inverse process. Near no flow boundaries one should be aware of possible nonuniqueness and the interactions of S and T.

EFFECT OF DATA ACCURACY

The results presented previously have been for hydraulic heads from the hypothetical model accurate to five decimal places. The obvious question is: How do errors in the hydraulic head affect the inverse process? In Figure 3 the relative error is plotted in % for the transmissivity calculations at each node for varying accuracies of the hydraulic head. R is the rounding index. For example R = 1.0 means the data have been rounded to the nearest foot and R = .01 means the data are accurate to the nearest .01 of a foot. Notice that for the last four node points where the sensitivity is the greatest, the error is less than 2% even if the data are rounded to the nearest foot. The maximum error is about 30% and occurs at node one, which has the lowest sensitivity. For data accuracies of .1 foot or better the error in transmissivity is about 2% or less for all except the first node point. Notice that even for five decimal places of accuracy the error at node one is still about 7% due to its low sensitivity.

Figure 4 shows the effect of data accuracy on the storativity calculations. It appears that the storativity in our hypothetical model is more sensitive to data accuracy than the transmissivity. For R = 1.0 the maximum error is about 35% but the error is sizable for most node points. The high error at the larger number nodes is due to low sensitivity, as shown in Figure 2. The large error near node one is due to the low sensitivity with respect to transmissivity and to the nonuniqueness problem discussed earlier. For all rounding options shown in Figure 4 the value of S/T at node one is within about 1% of the correct value. The error in storativity is less than 14% if the data are accurate to the nearest .1 foot with nodes one and two having the greatest error. Excluding nodes one and two, the error in storativity is less than 4% for data accurate to at least .1 foot. Notice that even for five decimal places of accuracy there is 7% and 10% error in storativity at nodes one and two respectively, due to nonuniqueness.

Normally, one would expect that, even in low sensitivity areas, good values of the parameters T and S could be calculated if the head values are given accurately enough. Figures 3 and 4 suggest this is not the case near node one. The nonuniqueness problem keeps the error in the range of 5-10% even when very accurate values of head are given. In contrast, the low sensitivity for storativity near node 10 has been overcome by specifying increasingly accurate head values.

DISCUSSION AND SUMMARY

The fact that considerable error in the transmissivity and storativity may occur in areas of low sensitivity should not be looked upon as a failing of the inverse procedure. It is simply a fact that not all areas of the model have been stressed equally. Until additional head data become available to establish a minimum sensitivity level in all areas of the model it simply is not possible to accurately estimate the transmissivity and storativity everywhere. The main advantage of the present work is that areas of low sensitivity may be delineated by looking at the sensitivity coefficients or some combination thereof.

Areas of low sensitivity for transmissivity and storativity occur where $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$ respectively are small. Of course at steady state $\frac{\partial h}{\partial t} = 0$ and the storativity cannot be determined since the sensitivity U_S is identically zero. As shown in column 5 of Table 1, the inverse calculation of storativity may become unstable if one uses data only approaching steady state. However, the transmissivity distribution may be determined at steady state within the limits of the model sensitivity. In general, the model sensitivity to transmissivity is greater in areas of low transmissivity and is smaller in areas of larger transmissivity (for example, see equation 26, 29, 32, and 42 or McElwee and Yukler, 1978). A similar inverse proportionality between U_S and the storativity holds.

In the hypothetical model used here an initial flat head distribution ($\frac{\partial h}{\partial x} = 0$) was used. This means that any initial guess for T would satisfy the initial condition. Only when deviations from this initial flat surface are produced by model discharge or recharge is it possible for the inverse procedure to begin to estimate the transmissivity distribution. Obviously the sensitivity increases with time and drawdown. This is the reason the early time calculations of T and S shown in Table 1 are not very good. (If the initial head had not been flat, a steady state inverse procedure would have given an initial T distribution. The model sensitivity to changes in this initial T distribution would again increase with time and drawdown.) The middle time inverse calculations for T and S shown in Table 1 are the best because the drawdown is substantial in most areas of the model and because the model has not approached the new steady state.

In addition to problems with low sensitivity, the inverse process may experience problems due to a basic nonuniqueness near no flow boundaries. Since no flow boundaries are usually specified by $\frac{\partial h}{\partial x} = 0$, it is apparent that the sensitivity with respect to T is zero at the boundary and is greatly reduced at nearby nodes. This low sensitivity may cause considerable error in calculating T, which will in turn create considerable error in S since the inverse procedure is primarily sensitive to the ratio S/T very near the boundary.

The effect of data inaccuracy has been simulated by rounding the head values from a hypothetical model. The maximum error in the inverse calculation for T and S decreases as more accurate head data are used. However, it is found that in certain areas of the model the error cannot be reduced to near zero by using very accurate data (5 decimal places). This is due to low sensitivities and nonuniqueness that are inherent in the model. The inverse procedure should not be blamed for this residual error; the model being used is simply not completely specified by the available data.

A formalism has been outlined for calculating sensitivity coefficients for groundwater models. The sensitivity coefficients have been used in a least squares inverse procedure. The interpretation and diagnosis of the inverse procedure results can be greatly aided by a detailed look at the sensitivity coefficients. In particular, areas of low and high confidence can be delineated. It is expected that sensitivity coefficients will find other useful applications in groundwater modeling. In particular, stochastic analysis of groundwater flow may benefit from the use of sensitivity coefficients.

NOTATION

E	Squared error between observed and predicted head
$f(x)$	Arbitrary function of x
$\bar{f},\bar{g}$	Column vectors used in the inverse solution
H,H_1,H_2	Constant head values at some boundary
h	Hydraulic head
h^*	Perturbed head produced by a change in T or S
he	Experimentally measured hydraulic head
i,j,k	Spatial indices for numbering nodes, used as subscript
ℓ	Length transverse to the cross sectional model
m	Iteration index, used as superscript in parentheses
$N+1$	Total number of nodes in model
n	Time index, used as superscript
Q	Water flux, volume per unit time
R	Maximum value of x
S	Storage coefficient
s	Drawdown
T	Transmissivity
t	Time
U_S	Sensitivity coefficient with respect to storage
U_T	Sensitivity coefficient with respect to transmissivity
x	Cartesian coordinate
x'	Normalized Cartesian coordinate
x_i	Coordinate of i^{th} node, $x_i = i\Delta x$
$\bar{\bar{\alpha}},\bar{\bar{\beta}},\bar{\bar{\gamma}}$	Coefficient matrices used in the inverse solution
Δh	Change in head produced by change in T or S
ΔS	Change in storage coefficient

ΔT	Change in transmissivity
Δt	Time step
Δx	Node spacing
δ_{ij}	Kronecker delta
$\delta(x-x_o)$	Delta function
ε	Error in head measurement
$\Theta(x_o-x)$	Heaviside function

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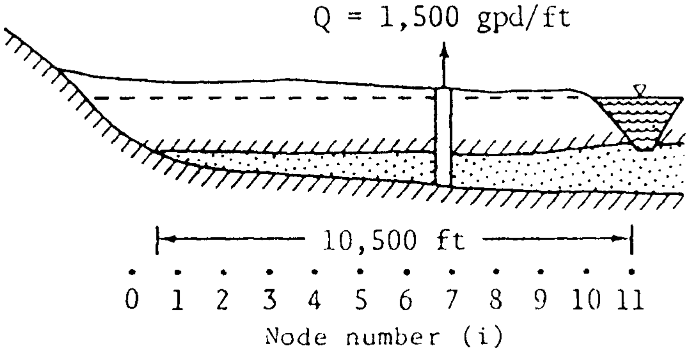
FIGURE LEGENDS

Figure 1	Hypothetical model
Figure 2	Model sensitivity to transmissivity and storage
Figure 3	Effect of data accuracy on calculated transmissivity
Figure 4	Effect of data accuracy on calculated storativity
Table 1	Inverse calculations over various time periods

HYPOTHETICAL MODEL



Node spacing is 1,000 ft

$T_{i+1/2} = (50,000 + i \cdot 2,000)$ gpd/ft

$T_{3/2} = 52,000$ gpd/ft

$S_i = .0045 + i \cdot 0.0005$

$S_1 = .0050$

Fig. 1.

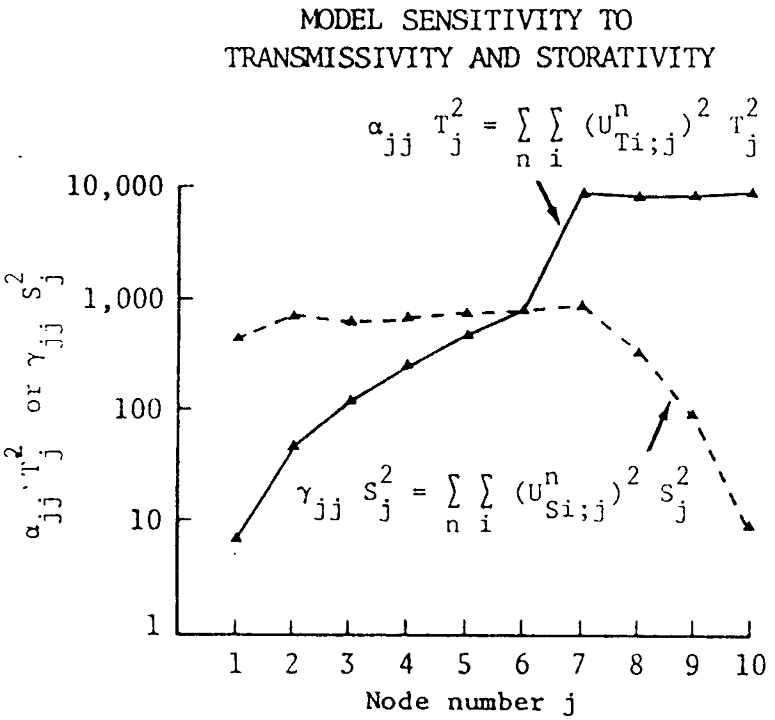

MODEL SENSITIVITY TO
TRANSMISSIVITY AND STORATIVITY
$\alpha_{jj} T_j^2 = \sum_n \sum_i (U^n_{Ti;j})^2 T_j^2$
$\gamma_{jj} S_j^2 = \sum_n \sum_i (U^n_{Si;j})^2 S_j^2$
$\alpha_{jj} T_j^2$ or $\gamma_{jj} S_j^2$
10,000
1,000
100
10
1
1
2
3
4
5
6
7
8
9
10
Node number j

Fig. 2.

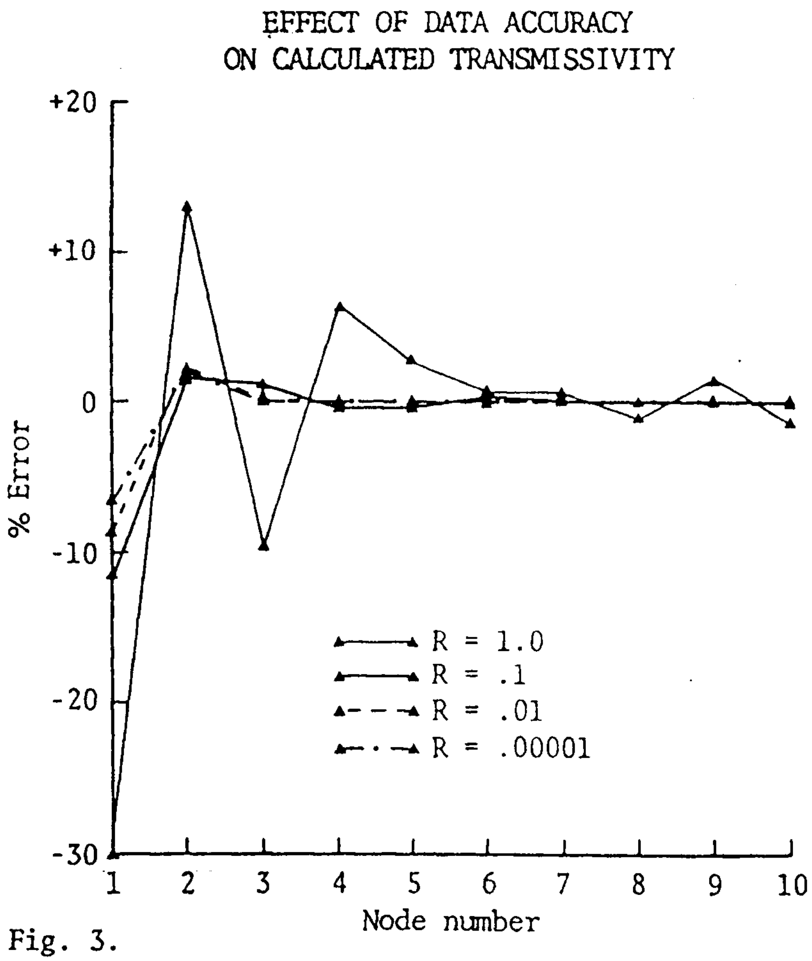

EFFECT OF DATA ACCURACY
ON CALCULATED TRANSMISSIVITY
+20
+10
0
-10
-20
-30
% Error
1
2
3
4
5
6
7
8
9
10
Node number
R = 1.0
R = .1
R = .01
R = .00001

Fig. 3.

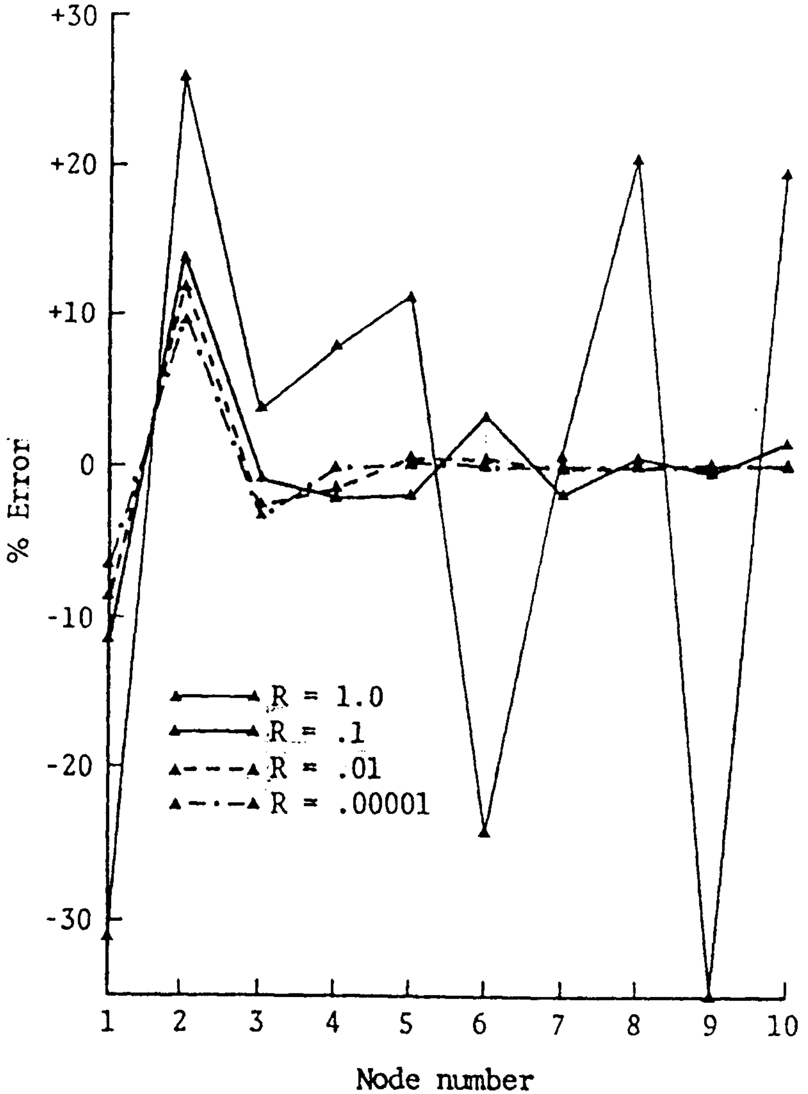

EFFECT OF DATA ACCURACY
ON CALCULATED STORATIVITY

Fig. 4.

APPENDIX

Numerical Solution of the Flow Equation

In general, numerical methods must be applied to find the solution to equation (43) (von Rosenberg, 1969; Carnahan, et al., 1969; Remson, et al., 1971). The Crank-Nicolson finite difference scheme dictates that equation (43) be evaluated at $x=x_i$ and $t=t^{n+1/2}$. A uniform grid system in space is assumed such that $x_{i+1}-x_i=\Delta x$. It may be convenient to accelerate the time step in order to approach the steady state more rapidly. In this case,

$$t^n = t^o + \Delta t \sum_{i=0}^{n-1} \alpha^i$$

$$t^n = t^o + \Delta t \frac{(1-\alpha^n)}{(1-\alpha)} \tag{A-1}$$

where t^n is the time after n time steps, t^o is the original starting time, Δt is the first time step, and α is the time step acceleration factor. α usually ranges from one to two in value. Half integer time values are given by

$$t^{n+1/2} = (t^{n+1} + t^n)/2 \tag{A-2}$$

The n+1 time step is simply

$$\Delta t^{n+1} = (\alpha)^n \Delta t \tag{A-3}$$

Notice that the space index is written as a subscript while the time index is written as a superscript (not to be confused as a power).

Evaluation of equation (43) at $x=x_i$ and $t=t^{n+1/2}$ by application of the difference operator, equation (46), yields

$$T_{i+1/2}(h_{i+1}^{n+1/2}-h_i^{n+1/2}) - T_{i-1/2}(h_i^{n+1/2}-h_{i-1}^{n+1/2}) = \frac{S_i(\Delta x)^2}{\Delta t^{n+1}}(h_i^{h+1}-h_i^n) - \frac{Q_i\Delta x}{\ell} \qquad \text{(A-4)}$$

after multiplying through by $(\Delta x)^2$. The half-integer head values on the left are eliminated by the Crank-Nicolson approximation.

$$h_i^{n+1/2} = (h_i^{n+1} + h_i^n)/2 \qquad \text{(A-5)}$$

This approximation allows equation (A-4) to be cast into the standard form needed for application of the Thomas Algorithm.

$$A_i h_{i-1}^{n+1} + B_i h_i^{n+1} + C_i h_{i+1}^{n+1} = D_i \qquad \text{(A-6)}$$

$$A_i = T_{i-1/2} = (T_i + T_{i-1})/2 \qquad \text{(A-7)}$$

$$C_i = T_{i+1/2} = (T_{i+1} + T_i)/2 \qquad \text{(A-8)}$$

$$B_i = -A_i - C_i - 2(\Delta x)^2 S_i/\Delta t^{n+1} \qquad \text{(A-9)}$$

$$D_i = -A_i h_{i-1}^n - C_i h_{i+1}^n + A_i h_i^n + C_i h_i^n - 2(\Delta x)^2 S_i h_i^n/\Delta t^{n+1} - 2Q_i\Delta x/\ell \qquad \text{(A-10)}$$

Since initial values of the head are known, repeated solution of equation (A-6) by the Thomas Algorithm will give the head values for any time step, provided appropriate boundary conditions are given.

The two commonly used boundary conditions are flow specified and head specified. The boundary conditions will be specified at x=0 and x=R. For convenience, it will be assumed that the flow is specified at x=0 and that the head is specified at x=R. In order to handle the specified flow at x=0 with a central difference formula, assume that x=0 corresponds to the point midway between x_o and x_1. x_o is a "ficticious" point introduced for convenience. This means that $x_i=(i-1/2)\Delta x$. If $x_{N+1} = (N+1/2)\Delta x = R$, there are N independent values of head since h_o and h_{N+1} are determined by the boundary conditions. Considering the inverse problem, it is clear that these N independent values of head can be used to solve for at most N independent values of the aquifer parameters at each time step. This point is discussed in more depth in the body of the paper.

Suppose that, at x=0, Q/ℓ is the specified flux per unit transverse width of the model; and at x=R the head is specified to be H. These boundary conditions in equation form are

$$\frac{h_1 - h_o}{\Delta x} = -Q_{1/2}/(\ell T_{1/2}) \tag{A-11}$$

and

$$h_{N+1} = H \tag{A-12}$$

Equation (A-11) is given by a simple application of Darcy's Law. If equation (A-4) is written out for i=1 and $T_{1/2}(h_1-h_o)$ is replaced by equation (A-11), it is seen that A_1 does not appear in the final equation. If the boundary flux $Q_{1/2}$ is included in Q_1, the only modification of equations (A-6) through (A-10) necessary for i=1 is to set

$$A_1 = 0 \qquad \text{(A-13)}$$

This is required for the Thomas Algorithm solution anyway. Notice that $T_{1/2}$ no longer appears in the solution equations. There are N independent transmissivity values $T_{3/4}$. . . $T_{N+1/2}$. Writing equation (A-4) out for i=N and replacing h_{N+1} by equation (A-12) gives

$$A_N h_{N-1}^{n+1} + B_N h_N^{n+1} = D_N - C_N H \qquad \text{(A-14)}$$

There are only two unknowns in equation (A-14); since $C_N H$ is known, it has been transposed to the right side of the equation. Equations (A-6) through (A-10) along with equations (A-13) and (A-14) form a set of N simultaneous equations in tridiagonal form as required for a solution with the Thomas Algorithm.

Numerical Solution of the Sensitivity Equations

As mentioned in the body of the paper, the numerical solution of the sensitivity equations very closely follows the numerical solution of the flow equation. Equations (45) and (51) are the sensitivity equations for $U_T(x,t;x_o)$ and $U_S(x,t;x_o)$, respectively. It was shown in the body of the paper how to deal with the delta function terms when numerical methods are used. This section will simply show how to use the Thomas Algorithm to solve for U_S and U_T.

Applying finite difference techniques to evaluate equation (45) at $x=x_i$, $x_o=x_{j+1/2}$, and $t=t^{n+1/2}$ yields

$$T_{i+1/2}(U^{n+1/2}_{Ti+1;j} - U^{n+1/2}_{Ti;j}) - T_{i-1/2}(U^{n+1/2}_{Ti;j} - U^{n+1/2}_{Ti-1;j}) + (h^{n+1/2}_{i+1} - h^{n+1/2}_{i})\delta_{i,j}$$

$$- (h^{n+1/2}_{i} - h^{n+1/2}_{i-1})\delta_{j,i-1} = \frac{S_i(\Delta x)^2}{\Delta t^{n+1}}(U^{n+1}_{Ti;j} - U^{n}_{Ti;j}). \qquad \text{(A-15)}$$

Equation A-15 may be derived an alternate way by employing the definition

$$U^{n}_{Ti;j} = \frac{\partial h^{n}_{i}}{\partial T_{j+1/2}} \qquad \text{(A-16)}$$

and simply differentiating the flow equation, (A-4), with respect to $T_{j+1/2}$. Use of the Crank-Nicolson approximation,

$$U^{n+1/2}_{Ti;j} = (U^{n+1}_{Ti;j} + U^{n}_{Ti;j})/2 \qquad \text{(A-17)}$$

allows equation (A-15) to be cast into the form needed for the Thomas Algorithm.

$$AT_{i;j}\, U^{n+1}_{Ti-1;j} + BT_{i;j}\, U^{n+1}_{Ti;j} + CT_{i;j}\, U^{n+1}_{Ti+1;j} = DT_{i;j} \tag{A-18}$$

$$AT_{i;j} = A_i = T_{i-1/2} \tag{A-19}$$

$$CT_{i;j} = C_i = T_{i+1/2} \tag{A-20}$$

$$BT_{i;j} = B_i = -A_i - C_i - 2(\Delta x)^2 S_i/\Delta t^{n+1} \tag{A-21}$$

$$\begin{aligned} DT_{i;j} = {} & -A_i U^n_{Ti-1;j} - C_i U^n_{Ti+1;j} + [A_i + C_i - 2(\Delta x)^2 S_i/\Delta t^{n+1}] U^n_{Ti;j} \\ & -2(h^{n+1/2}_{i+1} - h^{n+1/2}_{i})\delta_{i,j} + 2(h^{n+1/2}_{i} - h^{n+1/2}_{i-1})\delta_{i-1,j} \end{aligned} \tag{A-22}$$

Notice that of all the coefficients appearing in (A-18) only DT is different from the coefficients appearing in the flow equation, (A-6). In fact, DT is different only in that U_T appears instead of h and the fluxes, Q's, are replaced by the terms involving the Kronecker deltas. Therefore, the same computer code used to solve the flow equation can be used to solve the sensitivity equation. However, the computer time and memory requirements have increased considerably since equations (A-18) through (A-22) must be solved for the N different values of $j(1 \leq j \leq N)$.

It remains to impose the proper boundary conditions on U_T. The boundary conditions on the head are given by equations (A-11) and (A-12). Recall that the flux is specified at x=0 and the head is specified at x=R. The appropriate boundary conditions on the sensitivity, U_T, can be found by differentiating equations (A-11) and (A-12).

$$U_{T1;j}-U_{T0;j} = \frac{\partial h_1}{\partial T_{j+1/2}} - \frac{\partial h_0}{\partial T_{j+1/2}} = \frac{Q_{1/2}\Delta x}{\ell T_{1/2}^2}\,\delta_{j,0} \tag{A-23}$$

$$U_{T1;j}-U_{T0;j} = 0 \text{ if } j \neq 0$$

$$U_{TN+1;j} = \frac{\partial h_{N+1}}{\partial T_{j+1/2}} = 0 \tag{A-24}$$

Since $T_{1/2}$ (or A_1) does not appear in the flow equation, there is no reason to consider j=0 in equations (A-18) through (A-22) or in equation (A-23). Writing out equation (A-15) for i=1 and using equation (A-23) reveals that $AT_{1;j}$ does not appear in the final equation. Therefore,

$$AT_{1;j} = 0. \tag{A-25}$$

Use of equation (A-24) in equation (A-18) for i=N yields

$$AT_{N;j}U^{n+1}_{TN-1;j} + BT_{N;j}U^{n+1}_{TN;j} = DT_{N;j}. \tag{A-26}$$

Again equations (A-18) through (A-22) and equations (A-25) and (A-26) form a set of N simultaneous equations in tridiagonal form suitable for solution by the Thomas Algorithm for each value of j ($1 \leq j \leq N$).

Similar considerations can be applied to U_S, the sensitivity with respect to storativity. Evaluating equation (51) at $x=x_i$, $x_o=x_{j+1/2}$, and $t=t^{n+1/2}$ gives

$$T_{i+1/2}(U^{n+1/2}_{Si+1;j}-U^{n+1/2}_{Si;j}) - T_{i-1/2}(U^{n+1/2}_{Si;j}-U^{n+1/2}_{Si-1;j})$$

$$= \frac{S_i(\Delta x)^2}{\Delta t^{n+1}} \cdot (U^{n+1}_{Si;j}-U^{n}_{Si;j}) + \frac{(\Delta x)^2}{\Delta t^{n+1}} (h^{n+1}_i-h^n_i)\delta_{i;j}. \qquad \text{(A-27)}$$

Alternatively, equation (A-27) may be derived by differentiating equation (A-4) with respect to S_j and utilizing the definition

$$U^n_{Si;j} = \frac{\partial h^n_i}{\partial S_j} \qquad \text{(A-28)}$$

Once again the Crank-Nicolson approximation

$$U^{n+1/2}_{Si;j} = (U^{n+1}_{Si;j} + U^n_{Si;j})/2 \qquad \text{(A-29)}$$

allows equation (A-27) to be cast into the following form.

$$AS_{i;j}U^{n+1}_{Si-1;j} + BS_{i;j}U^{n+1}_{Si;j} + CS_{i;j}U^{n+1}_{Si+1;j} = DS_{i;j} \qquad \text{(A-30)}$$

$$AS_{i;j} = A_i = T_{i-1/2} \qquad \text{(A-31)}$$

$$CS_{i;j} = C_i = T_{i+1/2} \qquad \text{(A-32)}$$

$$BS_{i;j} = B_i = -A_i - C_i - 2(\Delta x)^2 S_i/\Delta t^{n+1} \tag{A-33}$$

$$DS_{i;j} = -A_i U^n_{Si-1;j} - C_i U^n_{Si+1;j} + [A_i + C_i - 2(\Delta x)^2 S_i/\Delta t^{n+1}] U^n_{Si;j}$$

$$+ [2(\Delta x)^2/\Delta t^{n+1}](h^{n+1}_i - h^n_i)\delta_{i,j} \tag{A-34}$$

Again only DS is different from the coefficients appearing in the flow equation. In DS, U_S appears instead of h and the Q term has been replaced by the single term involving the Kronecker delta. The same computer code used for h and U_T may be used to solve for U_S for the N values of $j(1 \leq j \leq N)$.

The boundary conditions on U_S may be found by differentiating equations (A-11) and (A-12) with respect to $S_j(1 \leq j \leq N)$.

$$U_{S1;j} - U_{S0;j} = \frac{\partial h_1}{\partial S_j} - \frac{\partial h_0}{\partial S_j} = 0 \tag{A-35}$$

$$U_{SN+1;j} = \frac{\partial h_{N+1}}{\partial S_j} = 0 \tag{A-36}$$

These boundary conditions are analogous to those for U_T contained in equations (A-23) and (A-24). Therefore, the same conclusions hold for i=1 and i=N.

$$AS_{1;j} = 0 \tag{A-37}$$

$$AS_{N;j}U^{n+1}_{SN-1;j} + BS_{N;j}U^{n+1}_{SN;j} = DS_{N;j} \qquad \text{(A-38)}$$

Equations (A-30) through (A-34) together with (A-37) and (A-38) form a tridiagonal system of N simultaneous equations solvable by the Thomas Algorithm for each value of $j(1 \leq j \leq N)$.