A STUDY OF THE GROUNDWATER INVERSE PROBLEM USING SENSITIVITY ANALYSIS AND ONE-DIMENSIONAL MODELS

Carl D. McElwee
Kansas Geological Survey, The University of Kansas
Lawrence, Kansas 66044

Prepared for presentation at the
Spring Meeting of AGU
May 22-27, 1980
Toronto, Ontario, Canada

INTRODUCTION

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. We shall see that this is not true many times. T, S, and Q are respectively transmissivity, storativity, and flux of water in or out of the system. One-dimensional models depending only on one spatial coordinate (x) have been choosen 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 one-dimensional models should be applicable to two-dimensional models as long as the results are applied parallel to streamlines. In this paper Q(x,t) will be assumed to be known. The variation of the model response only to changes in T(x) and S(x) will be considered.

SENSITIVITY COEFFICIENTS

h is 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 $\Delta T(x_o)$. The symbol $\delta(x-x_o)$ represents the Dirac delta function. The sensitivity with respect to variations in transmissivity (U_T) is defined as the change in head over ΔT in the limit as ΔT goes to zero. This sensitivity coefficient tells how much the head will be changed at point x due to a change in transmissivity ΔT at point x_o. Since $\Delta T(x_o)$ is assumed small, a first order expansion may be employed to obtain h* in terms of h, U_T and ΔT. If the transmissivity is changed at more than one point, then the new head h* must be found by integrating over the area where T(x) is changed. Outside the region bounded by x_1 and x_2 it is assumed that the transmissivity is not changed.

A similar development for the sensitivity with respect to storativity (U_S) yields expressions for h* in terms of h, U_S, and ΔS. In this case the storativity has been changed by ΔS at point x_o. Once again integration is required if the storativity is changed over a region.

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.

GENERAL PROPERTIES OF SENSITIVITY COEFFICIENTS

The general form of the one-dimensional flow equation is shown in this slide. T_{MAX} and S_{MAX} are the maximum values of the transmissivity and storativity, respectively. $Q/\ell\Delta x$ is the water flux per unit area of the model. ℓ is the transverse length perpendicular to x and Δx is the length over which Q is evenly distributed, usually one node spacing. Q is the volume of water per unit time as input or output to the model. The head can be written symbolically as depending upon the five quantities shown. If Q and the boundary conditions depend upon time, additional time dependence may be introduced.

Notice that at steady state the dependence on T_{MAX}/S_{MAX} disappears. In the homogeneous case the dependence on $T(x)/T_{MAX}$ also disappears. The final dependence on T is through the flux Q and disappears if there is no specified flux. If all three of these conditions are met then U_T is zero and the model doesn't depend on T.

Of course U_S is always zero at steady state.

In the homogeneous case when there are not specified fluxes, it is not difficult to show that the two sensitivity coefficients U_T and U_S are not independent. This means any T and S with the same ratio will give a good solution. In this case the inverse problem is non-unique.

Even if one allows spatial variation in T and S, the inverse problem is still non-unique since any S_{MAX} and T_{MAX} having the same ratio will give an equally good solution provided there are no specified fluxes. Theoretically, a specified flux at one point will uniquely determine the transmissivity and storativity distribution.

It is logical to use the sensitivity coefficients in developing an inverse process for groundwater modeling. 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 has simply 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 some aquifer parameters. By calculating and examining the sensitivity coefficients an indication of the stability of the inverse process may be obtained.

DIFFERENTIAL EQUATION FOR U_T

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 first equation in this slide. h* is the new head that results when the transmissivity is changed by ΔT at x_o. Applying the definition of U_T, a partial differential equation for U_T can be derived by subtracting the two equations, dividing by ΔT and taking the limit as ΔT approaches zero. The resulting partial differential equation for U_T looks very much like the original flow equation except for two differences. First, the fluxes do not appear; and second, there is an additional term involving the differentiation of a delta function.

Except in the simplest cases, numerical methods must be used to find U_T. The same solution techniques used for the flow equation may be used. U_T with a time index (n) as a superscript and two node indices as subscripts represents the change in head at point i at time n for a change in the transmissivity at $j+\frac{1}{2}$. T is specified midway between nodes; that is why ½ has been added to j. The delta function term is evaluated by simply applying the usual central difference scheme twice. $\delta_{i,j}$ is the Kronecker delta symbol. The h's are known from solution of the flow equation.

The partial differential equation for U_S is obtained in a manner similar to that for U_T. Once again the resulting equation looks like the flow equation except there are no fluxes and the delta function term has been added. For a numerical solution, $U^n_{Si;j}$ represents the change in head at time n and node point i for a change in storativity at node j. The delta function term is evaluated by the usual central difference approximation. The resulting numerical equation can be solved using the same techniques as used for the flow equation.

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. 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. From an analysis of the flow equations it is clear that $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$ are the important quantities; 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 transmissivity and storativity; consequently, the direct inverse process may have difficulty. Error in the head values will be more critical in regions where $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$ are small; because the error may be of the same order of magnitude as the partials. If this is the case, the partials will be very poorly represented and the transmissivity and storativity calculated in these regions will be greatly in error.

LEAST SQUARES INVERSE PROCEDURE

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 flow equations over any specific time interval. Rather, the best average solution is obtained over the historical period of record. 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 the first equation in this slide.

If h_{ei}^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 h_e. The error functional chosen to be minimized is the sum of the squared errors over all node points and time steps, as shown by the second equation in this slide. A necessary condition for minimization of the error is that the partial derivatives with respect to ΔT_j or ΔS_j be zero. This results in a system of 2N equations and 2N unknowns. Any standard solution technique may be used to obtain the ΔT's and ΔS's which minimize the error functional.

Unless the initial estimates for T and S are within about 20% of their correct values, the new aquifer parameters calculated the first time may not be good enough. The whole procedure may be repeated to obtain the next iteration values of ΔT_j and ΔS_j. 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 or the model is insensitive in certain areas, the procedure may not converge.

HYPOTHETICAL MODEL

This slide shows a hypothetical one-dimensional model chosen to illustrate the inverse procedure. The model has a constant head boundary on the right and a barrier boundary on the left. The initial head distribution is flat. The aquifer is being pumped at a rate of Q per unit transverse length at a distance of 3,000 feet from the constant head boundary. The distance between the two boundaries is 10,500 feet and 10 node points are used (1 is nearest the barrier boundary and 10 is nearest the constant head boundary). The transmissivity and storativity are assumed to increase linearly from the barrier boundary to the constant head boundary. The end values are shown on the slide. 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 procedure. 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.

TRANSMISSIVITY CALCULATIONS OVER VARIOUS TIME PERIODS

The correct values for the transmissivity at the 10 node points are shown in the second column of this slide. The initial estimate for transmissivity was 61,000 gpd/ft and for storativity was .00725. The transmissivity calculated for early time by the inverse procedure is shown in the third column. For these early times the drawdown at the well is less than 19 feet and the drawdown becomes less than one foot farther than three node points away from the well. The values of calculated transmissivity are within 20% of the actual values but there is no clear evidence that the inverse procedure has been successful in finding the correct values for transmissivity. Although they are not shown here similar comments can be made about the storativity calculations. The reason for this is that at early time periods the drawdown is small and the model is fairly insensitive to the transmissivity and storativity. This can be seen very easily by having the sensitivity coefficients printed out.

At middle times, shown in column 4, when the drawdown is substantial and hydarulic heads are changing fairly rapidly with time, the greatest sensitivity and best inverse solution results. The largest error in transmissivity is less than 7% and most are very close to the correct values. The storativity calculations, which are not shown, have less than 10% error and most are very close to the correct values.

The last column in this table shows the transmissivity calculations as the model approaches steady state. The storativity calculations have become unstable and cannot be made due to low sensitivity. The transmissivity calculations for the last four node points are very good. However, the calculated transmissivities for the first six node points are poor. This can be explained by looking at the sensitivity coefficients. The sensitivity at the last four nodes is about four orders of magnitude greater than for the first six nodes. This is because $\frac{\partial h}{\partial x}$ is practically zero for the first six node points.

MODEL SENSITIVITY TO TRANSMISSIVITY

Notice that for middle times the largest error in transmissivity occurs at node one and steadily decreases at higher number 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_T for each time step. A good compromise is to look at the diagonal elements of the system of equations to be solved for the ΔT's and ΔS's. These are shown as a_{jj} in this slide for the sensitivity with respect to transmissivity. The a_{jj} give a good indication of the total model sensitivity to the transmissivity at node j. Notice that indeed the lowest sensitivity occurs at node one and is about three orders of magnitude smaller than the sensitivity for the last four nodes. Examining these diagonal elements, a_{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.

EFFECT OF DATA ROUNDING

The results presented previously have been for hydraulic heads accurate to five decimal places. The obvious question is: how do errors in the hydraulic head affect the inverse process? On this slide we have plotted the absolute value of the relative error in % for the transmissivity calculations at each node for varying accuracies of the hydraulic head. R is the rounding number. For example R=1.0 means the data has been rounded to the nearest foot and R=.01 means the data is 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 is 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 accuracy the error at node one is still about 7% due to its low sensitivity.

The final slide shows the storativity calculations. It appears that storativity is more sensitive to data accuracy. For R=1.0 the maximum error is about 35% but the error is sizable for most node points. The error is less than 14% if the data is accurate to the nearest .1 foot with nodes one and two having the greatest error. The error is less than 4% at all other nodes.

CONCLUSION

The fact that considerable error in the transmissivity and storage 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 procedure is that areas of low sensitivity can be delineated.

SENSITIVITY COEFFICIENTS FOR TRANSMISSIVITY

$$h = h(x,t;T(x), S(x), Q(x,t))$$

$$h^* = h^*(x,t;T(x) + \delta(x-x_o)\Delta T(x_o), S(x), Q(x,t))$$

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

$\delta(x-x_o)$ is Dirac Delta Function

To first order in $\Delta T(x_o)$:

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

If T is varied between x_1 and x_2, must integrate

$$h^* \cong h + \int_{x_1}^{x_2} U_T(x,t;x_o)\Delta T(x_o)\,dx_o$$

SENSITIVITY COEFFICIENTS FOR STORATIVITY

$$h = h(x,t;T(x),S(x),Q(x,t))$$

$$h^* = h^*(x,t;T(x),S(x)+\delta(x-x_o)\Delta S(x_o),Q(x,t))$$

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

$\delta(x-x_o)$ is Dirac Delta Function

To first order in $\Delta S(x_o)$:

$$h^* \cong h + U_S(x,t;x_o)\Delta S(x_o)$$

If S is varied between x_1 and x_2, must integrate

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

GENERAL PROPERTIES OF SENSITIVITY COEFFICIENTS

The flow equation can be written:

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

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

U_T and U_S also have similar dependence

DIFFERENTIAL EQUATION FOR U_T

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

$$\frac{\partial}{\partial x}\left[\left(T(x) + \delta(x-x_0)\,\Delta T(x_0)\right)\frac{\partial h^*}{\partial x}\right] = S(x)\,\frac{\partial h^*}{\partial t} - \frac{Q(x)}{\ell\,\Delta x}$$

Subtracting, Dividing by $\Delta T(x_0)$, Taking limit gives:

$$\frac{\partial}{\partial x}\left[T(x)\,\frac{\partial U_T}{\partial x}\right] + \lim_{\Delta T(x_0)\to 0}\frac{\partial}{\partial x}\left[\delta(x-x_0)\,\frac{\partial h}{\partial x}\right] = S(x)\,\frac{\partial U_T}{\partial t}$$

NUMERICAL SOLUTION FOR U_T

$$U_{T\,i;j}^{\,n} = \frac{\partial h_i^n}{\partial T_{j+1/2}}$$

i, j are node indices
n is a time index

$$\frac{\partial}{\partial x}\left[\delta(x-x_0)\frac{\partial h}{\partial x}\right]_{\substack{x=x_i \\ x_0=x_{j+1/2}}}^{t=t^n} = \left[(h_{i+1}^n - h_i^n)\,\delta_{i,j} - (h_i^n - h_{i-1}^n)\,\delta_{i-1,j}\right]\Delta x^{-}$$

Use same solution technique as for flow equation.

DIFFERENTIAL EQUATION FOR U_s

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

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

Subtracting, Dividing by $\Delta S(x_o)$, Taking limit gives:

$$\frac{\partial}{\partial x}\left[T(x)\frac{\partial U_s}{\partial x}\right] = S(x)\frac{\partial U_s}{\partial t} + \delta(x-x_o)\frac{\partial h}{\partial t}$$

NUMERICAL SOLUTION FOR U_s

$$U_{s\,i;j}^{\,n} = \frac{\partial h_i^n}{\partial S_j}$$

i, j are node indices

n is a time index

$$\left[\delta(x-x_0)\frac{\partial h}{\partial t}\right]_{\substack{x=x_i \\ x_0=x_j}}^{t=t^{n+1/2}} = \left(h_i^{n+1} - h_i^{n}\right)\delta_{i,j}/\Delta t$$

Use same solution technique as for flow equation.

THE INVERSE PROBLEM

$\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$ are the important quantities.

Inverse process fails if they are zero.

Inverse process has difficulty if they are small.

Errors in head data are more critical

if $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial t}$ are small.

LEAST SQUARES INVERSE PROCEDURE

$$h_i^{*n} = h_i^n + \sum_j \left[U_{T\,i;j}^{n} \Delta T_j + U_{S\,i;j}^{n} \Delta S_j \right]$$

Let he_i^n be known historical head data.

$$\text{ERROR}(\Delta T_j, \Delta S_j) = \sum_n \sum_i \left[he_i^n - h_i^{*n} \right]^2$$

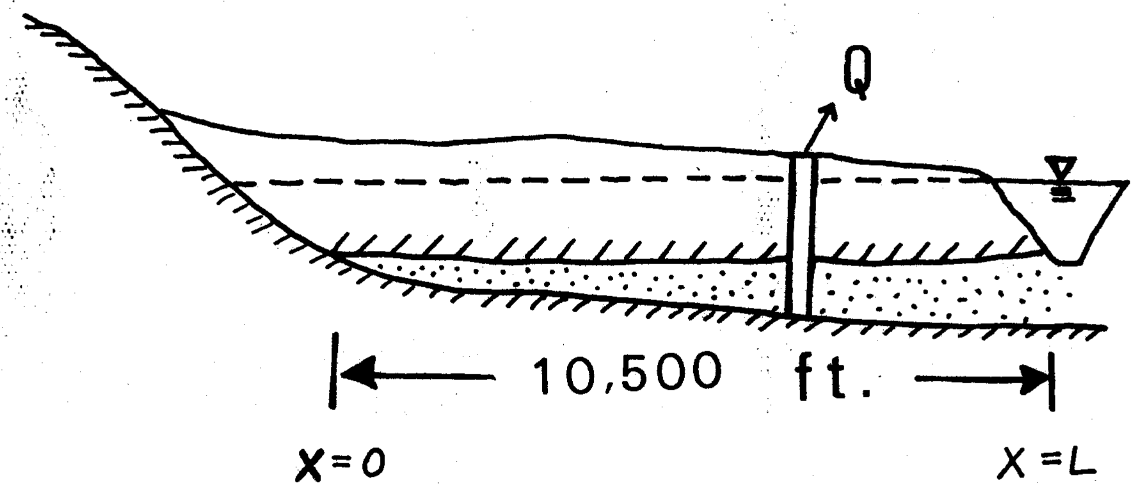
Minimize difference between he_i^n and h_i^{*n}.

$$\frac{\partial\, \text{ERROR}}{\partial \Delta T_j} = 0 \quad \text{and} \quad \frac{\partial\, \text{ERROR}}{\partial \Delta S_j} = 0 \qquad 1 \le j \le N$$

System of 2N equations and 2N unknowns.
$\Delta T_1, \cdots, \Delta T_N, \Delta S_1, \cdots, \Delta S_N$

Iterate until these are sufficently small.

HYPOTHETICAL MODEL



$T(0) = 52{,}000$ gpd/ft

$T(L) = 70{,}000$ gpd/ft

$T(X) = T(0) + aX$

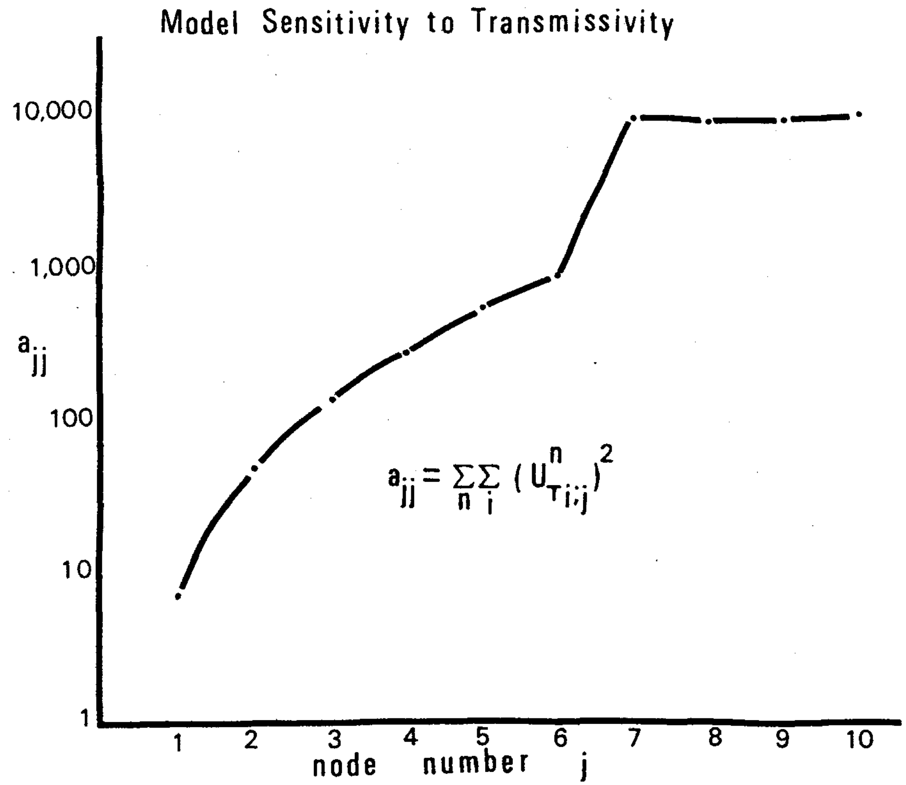
$S(0) = .0050$

$S(L) = .0095$

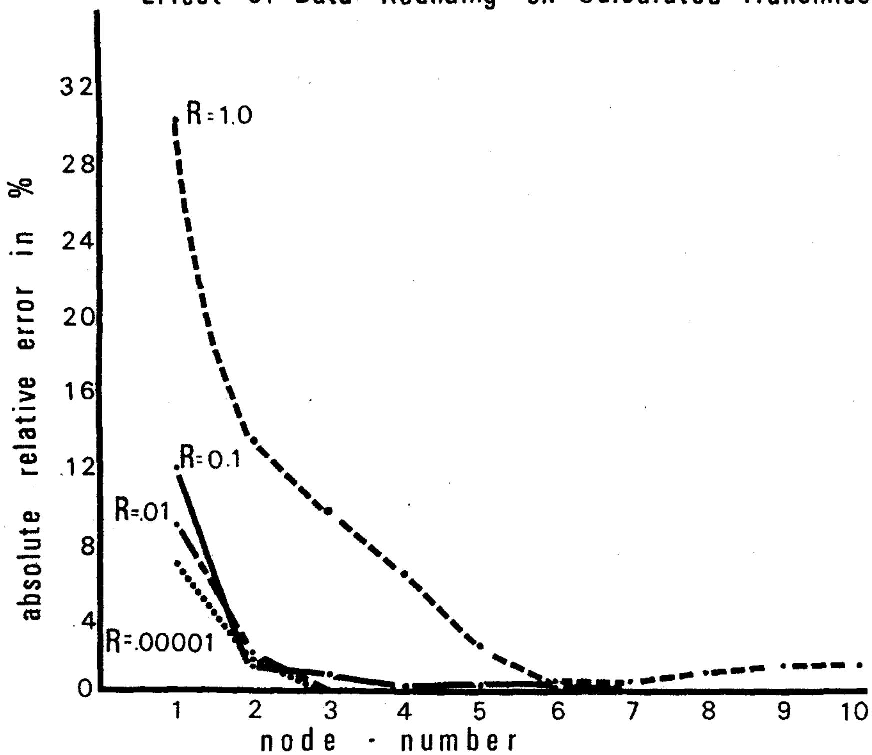
$S(X) = S(0) + bX$

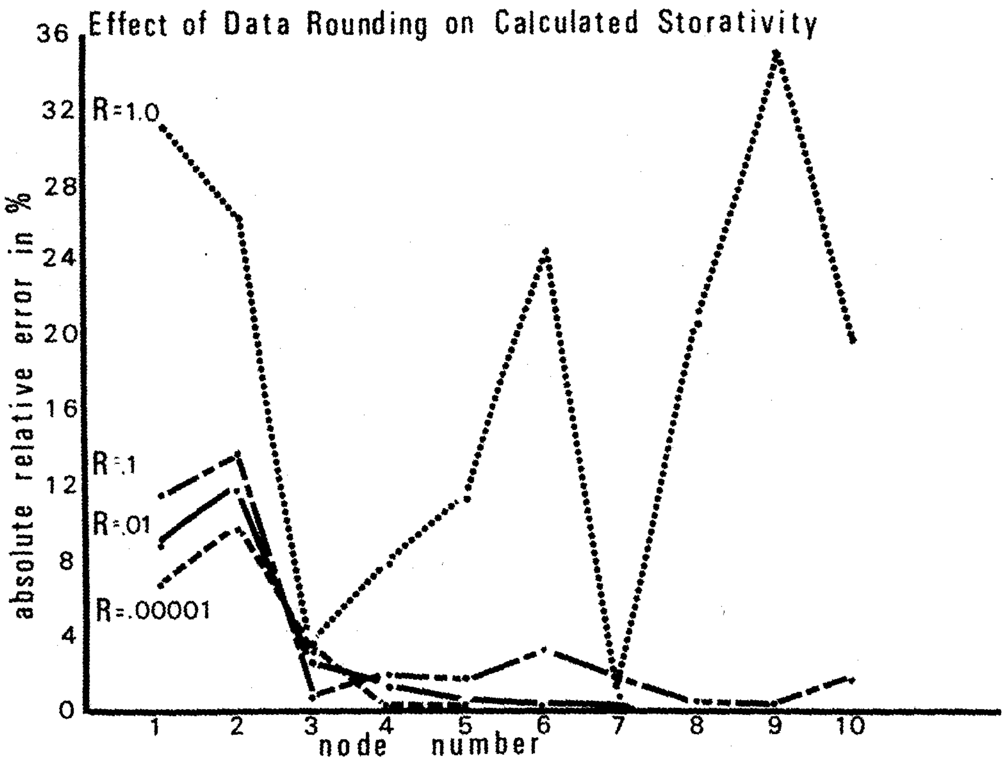
TRANSMISSIVITY CALCULATIONS OVER VARIOUS TIME PERIODS

GRID NUMBER	CORRECT VALUE	EARLY TIME	MIDDLE TIME	LATE TIME
1	52,000	59,575	48,415	59,473
2	54,000	62,107	55,064	57,934
3	56,000	64,365	55,980	53,250
4	58,000	66,684	57,955	50,500
5	60,000	69,070	60,000	49,681
6	62,000	71,283	62,002	21,853
7	64,000	55,152	64,001	63,988
8	66,000	56,931	66,000	66,004
9	68,000	58,603	68,000	68,005
10	70,000	60,330	70,000	70,005


Model Sensitivity to Transmissivity
10,000
1,000
100
10
1
a jj
$a_{jj} = \sum_n \sum_i (U^n_{T i;j})^2$
1 2 3 4 5 6 7 8 9 10
node number j

Effect of Data Rounding on Calculated Transmissivity





Effect of Data Rounding on Calculated Storativity
absolute relative error in %
36
32
28
24
20
16
12
8
4
0
R=1.0
R=.1
R=.01
R=.00001
1
2
3
4
5
6
7
8
9
10
node number