Transmissivity Resolution Obtained from the Inversion of Transient and Pseudo-Steady Drawdown Measurements.

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ABSTRACT

A key aspect of estimating transmissivity distributions from pumping tests is the spatial resolution of the estimation. Some assumption of spatial structure is needed to make an inversion possible. Both the nature of groundwater flow and assumed structure cause a smeared estimate. This research is focused on the how information content of the data smears the estimate. The inversion procedure near the solution is approximated as iterative linear updates. Linear resolution analysis of the distributed sensitivity to transmissivity indicates the limit of detail possible from the inversion.

To enable this research, adjoint-sensitivity calculations were added to MODFLOW-2000. The adjoint-sensitivity calculations significantly speed the calculation of the sensitivity matrix.

To highlight the concepts, we use a homogeneous aquifer with known storativity. The analysis indicates resolution of transmissivity is finer near the pumping and monitoring wells than in the regions between wells. Transient data are highly redundant with respect to transmissivity information. Very early time data do provide different spatial information than later time data do.

INTRODUCTION

An important question in any endeavor is "How well can we do it?" This is often a very complicated question. Bounding the answer rather than answering it directly often turns a difficult question into one we can answer. Our endeavor is to estimate subsurface properties. Resolution analysis provides insight into how well we can estimate the properties. Resolution analysis is a common technique in the geophysical community (Menke, 1989; Tarantola, 1987). With the exception of Vasco *et. al.* (1997), resolution analysis has not received attention in the groundwater literature.

Resolution analysis uses a linear approximation of the dependence of measurements on estimated parameters to determine how the inversion estimates relate to the actual subsurface properties. This is truly a bounding analysis because we assume that our groundwater model is accurate and that the estimated parameters are close enough to correct that non-linearity can be ignored. We also partially neglect the influence of errors in the measurements used in the inversion.

In this paper, we consider the estimation of the distribution of transmissivity in a hypothetical aquifer from drawdown measurements in observation wells about a pumping well. The emphasis is on the resolution analysis not on a specific inversion procedure. As this is a conference on MODFLOW, the addition of the adjoint state method (Sun, 1994; Townley and Wilson, 1985) of calculating sensitives to MODFLOW-2000 (Harbaugh et al., 2000; Hill et al., 2000) and its use in this investigation is highlighted.

SENSITIVITY CALCULATIONS

The simulated hypothetical aquifer has a central region 12.9 m by 7.6 m of constant grid spacing of 0.25 m. Twelve wells are positioned in roughly concentric rings about the central well as shown in Figure 1. The central region is surrounded by a grid that expands with a growth ratio of 1.5 to 150 m. The grid extends beyond the central region far enough that no appreciable drawdown occurs at the boundary during the simulation period. A constant storativity of 0.3 is used. A uniform transmissivity of 0.0032 m^2 /s is used. A constant pumping rate of 5 l/s is maintained for 10,000 s (170 min). No appreciable drawdown occurs at the boundary during the simulation period. A total of 122 observations were made from drawdown at the wells. Four drawdown observations per log base ten time interval were recorded. Early observations, before a well responds, were not included.
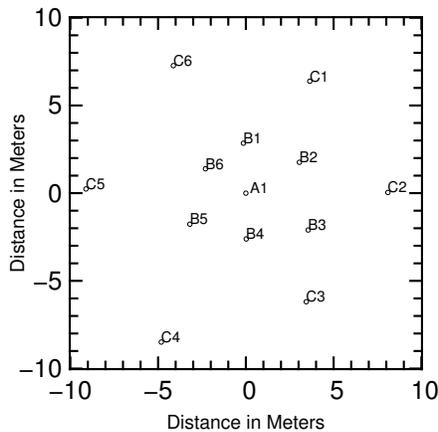
Figure 1 Well Field

The model has a total of 9409 cells. Estimating a distribution of transmissivity refers to allowing each cell of the MODFLOW model to be assigned a different value. As a consequence, a matrix of parameter sensitivities, the sensitivities of the drawdown observations to transmissivity, must be calculated for each cell in the model. Calculating the sensitivity matrix using the sensitivity equation process of MODFLOW-2000 requires a separate calculation for each cell. This calculation required 19 h on a 1 GHz PC. These calculations agree well with the analytic solutions presented by Oliver (1993). An adjoint states based calculation of drawdown sensitivity to hydraulic conductivity was added to MODFLOW-2000 following the procedure described in Carrera and Medina (1994).

The procedure of Carrera and Medina requires one adjoint states calculation per observation location. These calculations took 2.3 minutes. The calculations were not sufficiently accurate for our purpose. They disagree by 10% to 20% with the sensitivity equation based calculations. Errors were larger for cells with small sensitivity but these errors are not relevant. The inaccuracy may represent a coding error or a fundamental limitation. Improvements to the calculations are being investigated. While not sufficient for the resolution analysis, 20% accuracy may be acceptable for the early stages of an inversion where non-linearity makes any calculation inaccurate.

The adjoint sensitivity calculations that were used were based on a separate adjoint states calculation for each of the 122 observations. These calculations took 94 minutes to complete, 12 times faster than the sensitivity equation calculation. Errors for significant sensitives were less than 0.1% for observations that coincided with the end of a time step and between 0.1% and 2% for interpolated observations. Improvements to speed are anticipated. We have noted that if only the first third of the adjoint states calculation were performed an addition factor of three speed-up could be obtained without appreciable increase in error.

RESOLUTION MATRIX

The resolution matrix is based on the sensitivity calculation of the last step of a non-linear inversion procedure (Tarantola, 1987). At the last step the inversion can be linearized to

$$Gm = d \tag{1}$$

where G is the sensitivity matrix, m is an unknown error in the transmissivity parameters, and d is the difference between the observation with the current parameter estimates and the measured observations. If G could be inverted ,we could update the transmissivity estimate by $\Delta m = G^{-1}d$, but G is a 138 by 9409 matrix which does not have an inverse. Instead, we write the update as

$$\Delta m = G^{-g}d \tag{2}$$

G^{-g} is referred to as the generalized inverse. The update, Δm, can be related to the error, m, by combining 1 and 2.

$$\Delta m = G^{-g}Gm \tag{3}$$

$R = G^{-g}G$ is the resolution matrix (Menke, 1989; Tarantola, 1987). The resolution matrix describes how the transmissivity update is related to the transmissivity error. Because G^{-g} is not the inverse of G, the update is not equal to the error. It can be shown that, if the transmissivity estimate is nearly correct then non-linear effects are not important and equation 3 holds for the transmissivity estimate itself. That is,

$$T_{est} = RT_{true} \tag{4}$$

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where T_{est} is the transmissivity estimate of the inversion and T_{true} is the real transmissivity. Equation 4 neglects errors in the model, measurements errors, and other plagues of inversion. These caveats aside, the resolution matrix provides us with a tool that we can use to set our expectations, design experiments, and compare different inversion strategies.

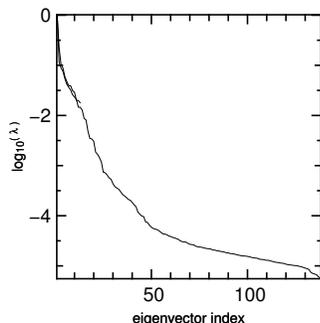## ANALYSIS USING TRUNCATED SINGULAR VALUE DECOMPOSITION

In equation 2, G^{-g} incorporates the constraints used in the inversion. These constraints may include prior information, regularization equations to impose a structure on the solution, or a prior covariance structure arising from a Bayesian formulation of the inversion problem. The constraints must be included in the resolution analysis of a particular inversion process. We simplify the analysis by using truncated singular value decomposition as the way of calculating the generalized inverse. Menke (1989) refers to this G^{-g} as the natural generalized inverse. It is natural because it constrains the estimated distribution to only have variations that are distinguishable from the measurements. Any form of regularization introduces a bias into the estimation. The bias of the truncated singular decomposition approach is based on the information content in the data. If a variation in transmissivity cannot be clearly supported by the data, it is left out of the solution.

Figure 2 Normalized eigenvalues obtained from singular decomposition of the sensitivity matrix.

The singular value decomposition of G results in

$$G = U\Lambda V^T \qquad (5)$$

where Λ is a diagonal matrix of eigenvalues, λ_i, and U and V are matrices containing the associated eigenvectors. We refer to U as the data eigenvectors and V as the transmissivity eigenvectors.

Because of the orthogonality and normality properties of U and V

$$G^{-g} = V\Lambda^{-1}U^T \qquad (6)$$

where Λ^{-1} is a diagonal matrix with diagonal elements $\frac{1}{\lambda_i}$. Very small eigenvalues indicate a redundancy in the information about the transmissivity contained in the observations. Two measurements with exactly the same information content would produce an eigenvalue with a value of zero.

Figure 2 plots the normalized eigenvalues from singular decomposition of the sensitivity matrix using a semi-log scale. The eigenvectors are normalized with respect to the largest eigenvalue. The figure shows a rapid decline in the eigenvalues implying a large redundancy in information. Two sets of eigenvalues are plotted. One using all the 138 observations and one using only the 13 observations acquired at 10,000 s, the last time step of the simulation. The eigenvalues of these 13 observations nearly coincide with the thirteen largest eigenvalues of the full data set. The overlap of the two sets suggests that observations from different locations provide much more new information than can be obtained by adding a large number of new observations at current locations, a conclusion that is supported by the resolution analysis presented below.

A consequence of small eigenvalues is that there are weighted combinations of transmissivity, Δm, that have a very small influence on the calculated drawdown observations. These combinations are defined by αV_i, where α is a constant. There is a corresponding weighted combination of drawdown measurements, d_i, defined by βU_i that are influenced by the V_i. If d_i is imperfect, as of course it will be using measured data, then the errors in d_i will be magnified by $\frac{1}{\lambda_i}$ in the resulting prediction of Δm_i. To avoid this problem, we truncate the singular value decomposition at some minimum λ_i. This is the method whereby only variations in transmissivity that can be supported by the data are retained. The appropriate truncation level is related to the uncertainty in the observations. Vogel (2003) provides an algorithm for selecting an appropriate truncation level.

RESOLUTION OF TRANSMISSIVITY ESTIMATES

The resolution matrix is large; number of parameters by number of parameters. The spread function provides one way of reducing the resolution matrix to a comprehensible level. Menke(1989, pg 68) defines the spread function for the resolution matrix as

$$\text{spread}(R) = \sum_{i=1}^{n} \sum_{j=1}^{n} (R_{ij} - I_{ij})^2 \tag{7}$$

where I is the identity matrix. We define the spread of each cell as

$$S_i = 1 - \sum_{j=1}^{n} (R_{ij} - I_{ij})^2 \tag{8}$$

A value of 1 for a cell implies that the cell can be estimated with good accuracy. It also implies that the estimate for the cell is not influenced by the transmissivity of other cells. A small value implies that the estimates of transmissivity for a cell are strongly influenced by other cells. A value near zero indicates the the transmissivity estimate for the cell will not related to the actual transmissivity of the cell.

Figure 3 plots the spread functions for three separate cases; a) using all the eigenvectors of the 138 observations, b) using the largest 29 eigenvectors, and c) using only the 13 observations acquired at the last time step of the simulation. The plots are color based and each plot is rescaled so that the largest values are purple and and small values are red. The color scale is drawn to the right of each plot. Cells with values below the cutoff on the color scale are not drawn.

(a)   (b)
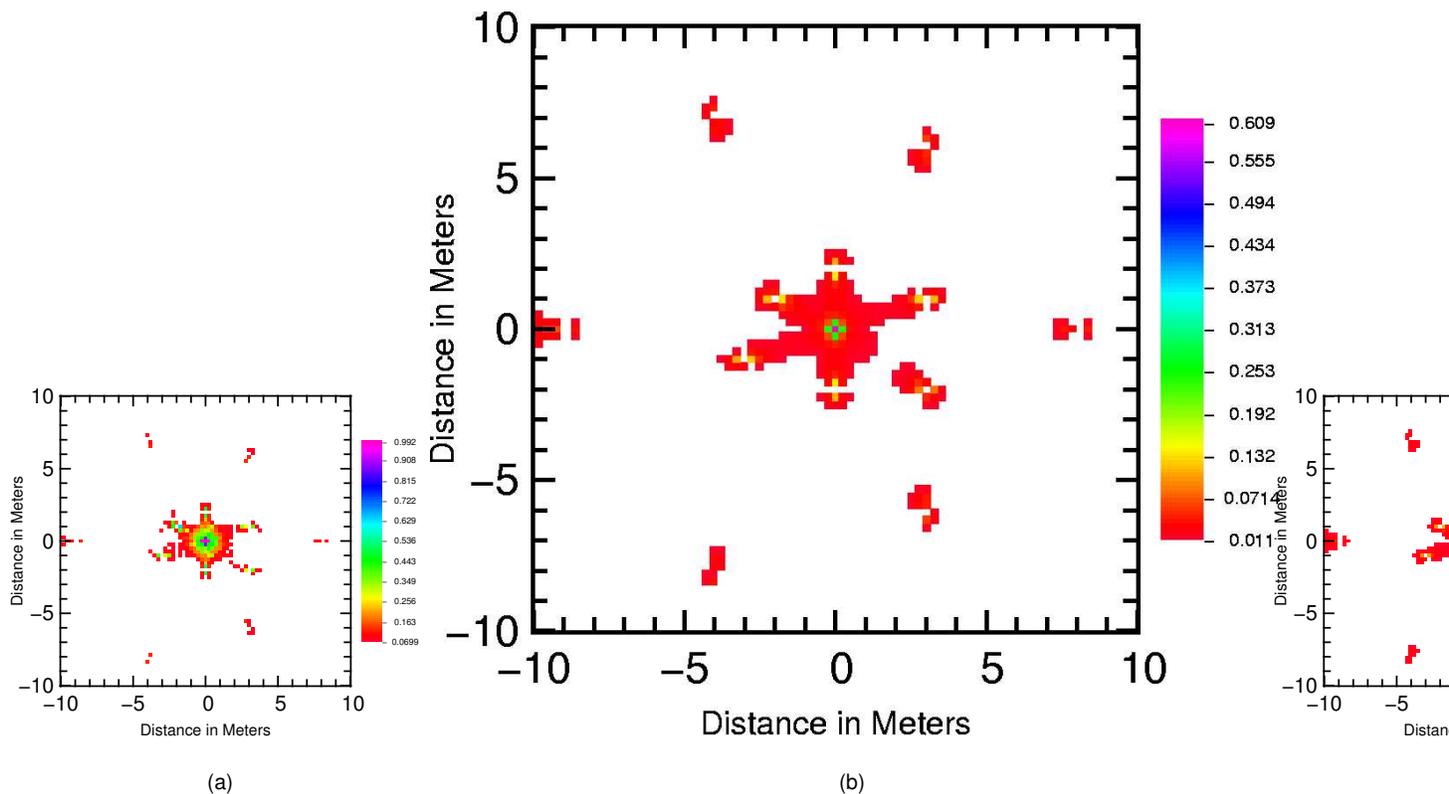
Figure 3 Spread functions of the resolution matrix. a) Using all the eigenvectors. b) Using eigenvectors of the 29 largest eigenvalues c) Using only 10,000 s observations.

Plot 3a would be appropriate if the eigenvalues were all approximately the same size indicating that all of the eigenvectors could be resolved by the inversion process. The plot shows values near 1 for the cells immediately adjacent to the pumping well and relatively large values in the vicinity of the well, indicating

that the transmissivity of a disturbed zone could be resolved at this grid size. Away from the well the spread function diminishes rapidly with only a 3 m diameter circle showing a strong anticipated correlation between the estimate and the actual local transmissivity. The cells immediately adjacent to the observation wells would also be correlated with their estimates. If observations were acquired more often, then a plot similar to plot 3a would indicate higher resolution, an unrealistic conclusion.

Plot 3b is more realistic. Only the 29 eigenvectors associated with normalized eigenvalues larger than 10^{-3} were used to create the spread function. The plot indicates that nowhere can transmissivity be resolved at the 25 cm scale of the grid. With a lower cutoff of 0.01, the large red area does not indicate a region of even moderate resolution. As with the eigenvalue comparison of the full observation set with just one observation at each well, a comparison of plots 3c to 3b indicates that the full set of observations only provides a small improvement as we concluded earlier from Figure 2.

One might conclude that transient data are not of value in estimating a transmissivity distribution. We do not believe that such a conclusion is justified. Investigations of the sensitivity matrix indicate that sensitivity is different during the early portion of the drawdown compared to the late portion and that the shape of the sensitivity field changes rapidly in this region. This suggests that more measurements at early times may be valuable. The crux of the matter lies in the signal to noise ratio of the measurements. A larger signal to noise ratio correlates with a lower eigenvalue cutoff, more retained eigenvectors and more finely determined transmissivity. Unfortunately, the most important data is related to small values of drawdown.
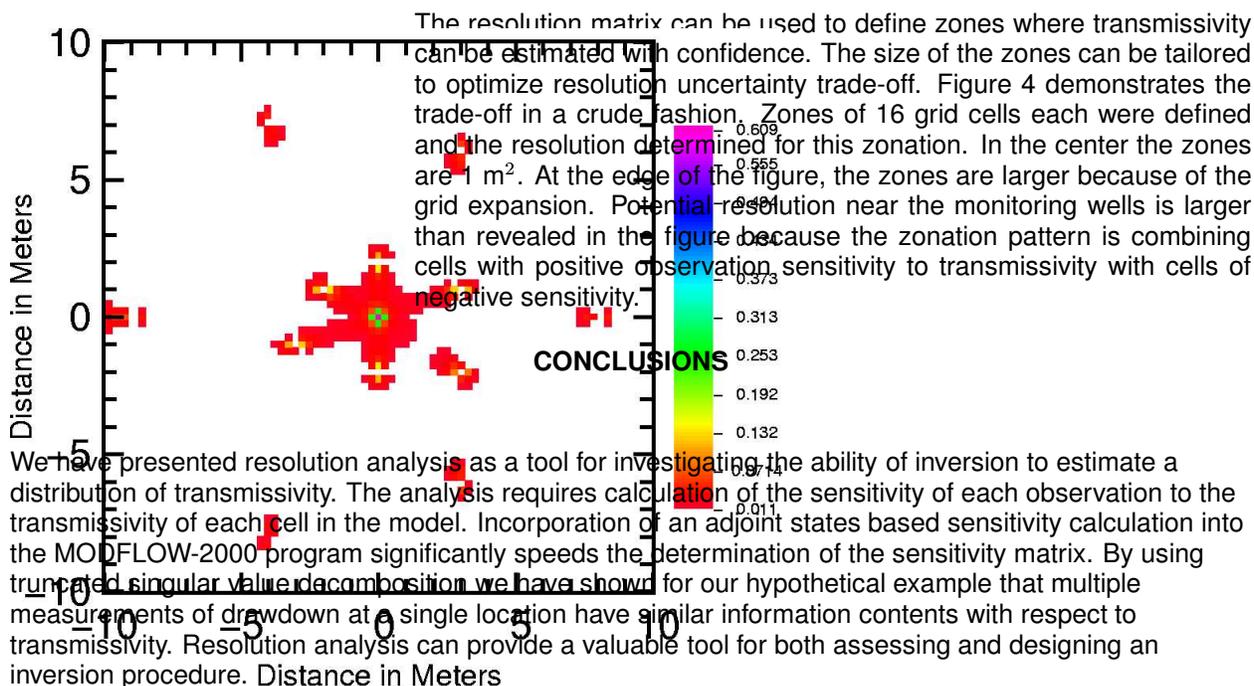
The resolution matrix can be used to define zones where transmissivity can be estimated with confidence. The size of the zones can be tailored to optimize resolution uncertainty trade-off. Figure 4 demonstrates the trade-off in a crude fashion. Zones of 16 grid cells each were defined and the resolution determined for this zonation. In the center the zones are 1 m^2. At the edge of the figure, the zones are larger because of the grid expansion. Potential resolution near the monitoring wells is larger than revealed in the figure because the zonation pattern is combining cells with positive observation sensitivity to transmissivity with cells of negative sensitivity.

CONCLUSIONS

We have presented resolution analysis as a tool for investigating the ability of inversion to estimate a distribution of transmissivity. The analysis requires calculation of the sensitivity of each observation to the transmissivity of each cell in the model. Incorporation of an adjoint states based sensitivity calculation into the MODFLOW-2000 program significantly speeds the determination of the sensitivity matrix. By using truncated singular value decomposition we have shown for our hypothetical example that multiple measurements of drawdown at a single location have similar information contents with respect to transmissivity. Resolution analysis can provide a valuable tool for both assessing and designing an inversion procedure.

Figure 4 Resolution for 1 m zones

ACKNOWLEGMENTS

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