GEOSTATISTICAL AND ADJOINT SENSITIVITY TECHNIQUES APPLIED TO A CONCEPTUAL MODEL OF GROUND-WATER FLOW IN THE PARADOX BASIN, UTAH

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ABSTRACT

Sensitivity and uncertainty analysis are important components of performance assessment activities for potential high-level radioactive waste repositories. The application of geostatistical and adjoint sensitivity techniques to aid in the calibration of an existing conceptual model of ground-water flow is demonstrated for the Leadville Limestone in Paradox Basin, Utah. The geostatistical method called kriging is used to statistically analyze the measured potentiometric data for the Leadville. This analysis consists of identifying anomalous data and data trends and characterizing the correlation structure between data points. Adjoint sensitivity analysis is then performed to aid in the calibration of a conceptual model of ground-water flow to the Leadville measured potentiometric data. Sensitivity derivatives of the fit between the modeled Leadville potentiometric surface and the measured potentiometric data to model parameters and boundary conditions are calculated by the adjoint method. These sensitivity derivatives are used to determine which model parameter and boundary condition values should be modified to most efficiently improve the fit of modeled to measured potentiometric conditions.

INTRODUCTION

As part of the licensing application for an underground high-level nuclear waste repository for a particular site, performance assessment calculations are required to demonstrate that the site complies with U.S. Environmental Protection Agency (EPA) standards[1] and U.S. Nuclear Regulatory Commission (NRC) regulations[2]. A calibrated conceptual model of the regional ground-water flow system in the vicinity of the site is required in order to conduct performance assessment calculations that pertain to ground-water flow and radionuclide transport. The calibration of ground-water flow models generally consists of fitting modeled potentiometric surfaces to measured potentiometric data through the adjustment of model parameters and boundary conditions. This paper demonstrates the use of geostatistical interpolation and adjoint sensitivity analysis in the calibration process.

Geostatistical and adjoint sensitivity analyses are performed to aid in the calibration of an existing conceptual model[3] of the regional ground-water flow system for Paradox Basin, Utah. Figure 1 shows the conceptual model boundaries with respect to rivers, cities and geologic features within Paradox Basin and the potential repository location at Davis Canyon. The flow system consists of three major geohydrologic units[3].

- An upper aquifer composed of Permian-age sandstones and shales.
- Pennsylvanian-age rocks that are generally of low permeability, including the Paradox Formation which would contain the repository horizon in the event that the Davis Canyon potential repository location is selected and licensed.
- A lower aquifer that is composed of the Leadville and Ouray Limestones and the Elbert Formation.

The Leadville-Ouray-Elbert, which is hereafter referred to as the Leadville, comprises the lower unit in the conceptual model of ground-water flow at Paradox Basin, and it is the geohydrologic unit of interest in this calibration exercise. Potentiometric head data[4] are available for the Leadville in Paradox Basin. The spatial distribution of these data points and the corresponding potentials in meters are shown in Fig. 2. The published potentiometric data for Paradox Basin[4] indicate that the hydraulic potential is downward across the Paradox Formation in the vicinity of Davis Canyon. Thus, the Leadville is important in the evaluation of Davis Canyon as a potential repository location, because the Leadville is the first major aquifer underlying the Paradox Formation. Within the boundaries of the conceptual model, the Leadville varies in thickness between 245 m and 335 m at depths below land surface ranging from 600 m to 3,700 m.

BACKGROUND

The geostatistical method called kriging[5] is used to statistically analyze the irregularly-spaced potentiometric data in Fig. 2. The objective of kriging the available potentiometric data is to gain a better understanding of the data and confidence in the data consistency. Kriging is used to identify anomalous data and data trends and to characterize the correlation structure between data points.

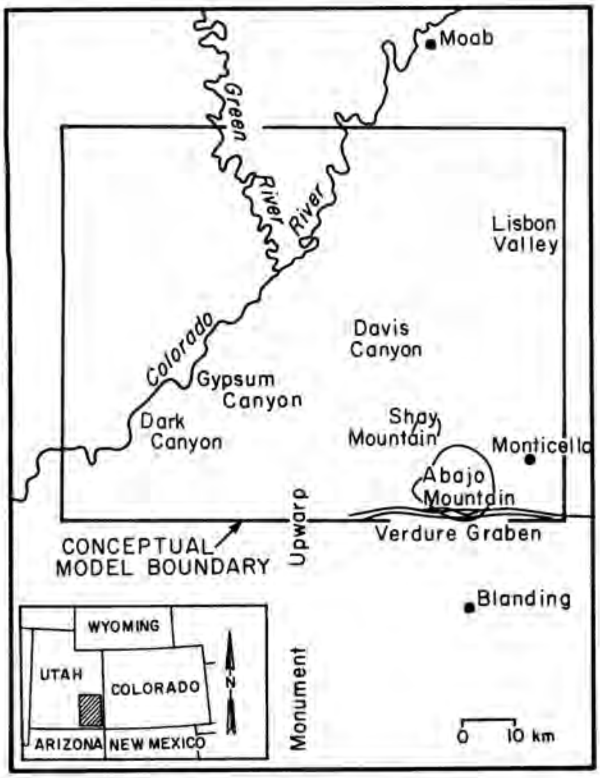

Fig. 1. Paradox Basin study area.

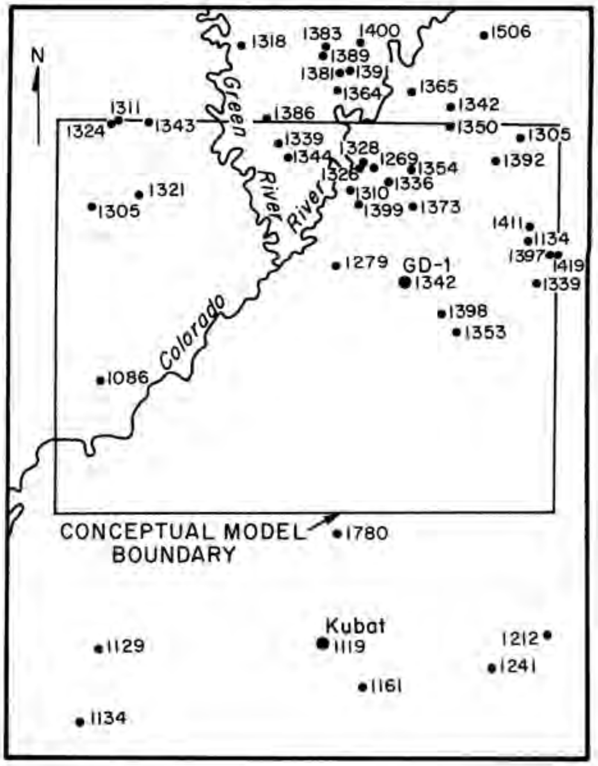

Fig. 2. Leadville potentiometric data.

Adjoint sensitivity analysis[6,7] is then performed to aid in the calibration of the existing conceptual model of ground-water flow as it pertains to the Leadville flow regime. A post-processor code has been developed to perform adjoint sensitivity calculations for SWENT[8], which is a three-dimensional, finite-difference, ground-water flow and radionuclide transport code. This post-processor for SWENT computes sensitivity derivatives or coefficients for selected measures of model performance, called performance measures, to model parameters and boundary conditions. The sensitivity coefficients are computed by the adjoint method and are exact derivatives of the performance measures with respect to the parameters and boundary conditions for the modeled system, taken about the assumed parameter and boundary condition values. The sensitivity coefficients represent the approximate percentage change that would occur in the performance measure for a 1 percent increase in the value of the model parameter or boundary condition. One performance measure that can be calculated is the average squared deviation between modeled and measured pressures, which is a measure of the fit between modeled potentiometric surfaces and measured potentiometric data. Thus, sensitivity coefficients for this performance measure can be used to systematically calibrate the conceptual model of ground-water flow to measured potentiometric data. The largest sensitivity coefficients direct the modeler's attention to parameters and boundary conditions that have the most influence on the fit of modeled to measured pressures, and these parameters and boundary conditions can be adjusted within their ranges of uncertainty to improve the fit.

GEOSTATISTICAL ANALYSIS OF POTENTIOMETRIC DATA

The geostatistical method called kriging was used to analyze the available Leadville potentiometric data. Potentiometric head values are usually predicted accurately from nearby data, and to a decreasing extent as the distance between the data and the location where potentiometric head is to be predicted increases. This phenomenon is referred to as spatial correlation, and the quantification of the spatial correlation of the measured data is the first step in geostatistics. This involves the development of semi-variograms that graphically display the spatial variability of the data as a function of distance and orientation (e.g., north-south). These directional semi-variograms aid in the identification of any trends (an overall pattern or drift) in the data. Directional semi-variograms (not shown) were developed for the available Leadville potentiometric data, and a polynomial trend surface was fit to the data to test for a trend. A linear trend was examined and was found to be statistically significant, whereas a quadratic trend did not improve the fit of the trend surface to the potentiometric data. The directional semi-variograms indicate that the trend is from the north-northeast to the south-southwest. The trend surface residuals from the linear plane were used to create a similiar, second set of semi-variograms. No other trends were apparent in this second set of semi-variograms. Figure 3 shows an overall (all directions) empirical semi-variogram (individual data points) of the linear residuals with a theoretical semi-variogram model (line) superimposed. A spherical model with a nugget of 1,400 m^2, sill of 7,400 m^2, and range of 70 km provided a reasonable fit to the trend surface residuals.

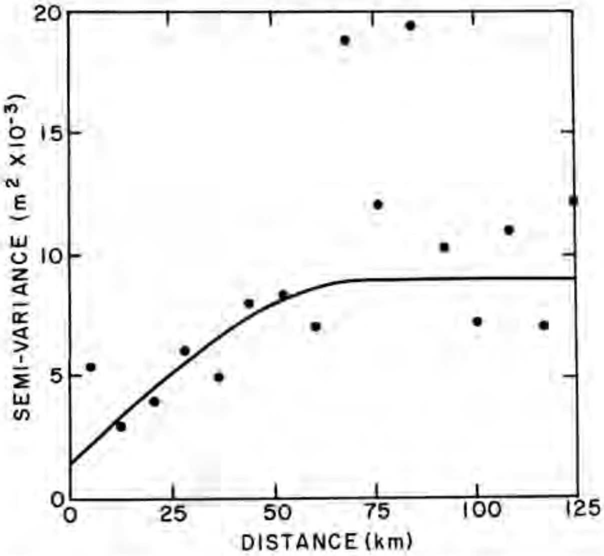

Fig. 3. Empirical and theoretical semi-variograms for the linear residuals.

Assuming that potentiometric measurements for a given location in the Leadville are normally distributed around the actual value, the nugget of 1,400 m^2 is equivalent to the measurement error variance. Thus roughly 95 percent of the reported potentiometric values are within 74 m (two times the square root of 1,400 m^2) of their respective actual values. The range of 70 km indicates that the potentiometric head data are correlated over separation distances as large as 70 m.

Cross-validation was performed on this theoretical model to determine the goodness of fit to the data. Cross-validation removes each point from the original data set and estimates it using kriging with the theoretical model. The difference between the actual and predicted value is then normalized by the kriging standard error, resulting in what are called standardized residuals. Caution should be used in blindly judging the goodness of fit solely on cross-validation statistics. A visual check of the semi-variogram model to the empirical data is even more important. Two extremely large standardized residuals (greater than 3 standard deviations) were identified through cross-validation. These were the standardized residuals for the potentiometric heads at the western end of Verdure Graben of 1,780 m and in Lisbon Valley of 1,134 m (see Figs. 1 and 2). These potentiometric heads must be considered with respect to the conceptual model of ground-water flow within the Leadville to evaluate whether or not there is a possible physical basis for these statistically anomalous potentiometric heads.

CONCEPTUAL MODEL OF GROUND-WATER FLOW IN THE LEADVILLE

The existing conceptual model for ground-water flow in Paradox Basin is essentially the same as that developed in 1982 and presented in INTERA[3], with the Paradox Formation explicitly included as a layer between the upper aquifer and the Leadville. Boundary conditions and the modeled spatial distribution of horizontal hydraulic conductivity (K_H) for the Leadville are shown in Fig. 4. The area shown is that identified by the conceptual model boundary in Figs. 1 and 2[3]. The base K_H value for the Leadville is 10^{-7} m/sec[3]. Modeled variations to this base K_H value are as follows[3]:

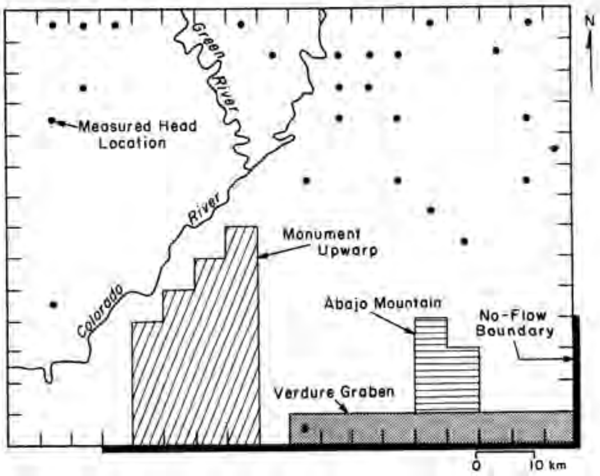

Fig. 4. Modeled boundary conditions and hydraulic conductivity zones for the Leadville.

- $K_H = 3\times10^{-7}$ m/sec in the Monument Upwarp area, due to fracturing that is believed to enhance K_H in this area.
- $K_H = 10^{-10}$ m/sec in the Abajo Mountains; a laccolith which is presumed to be of lower hydraulic conductivity than the Leadville.
- $K_H = 3\times10^{-6}$ m/sec in the Verdure Graben along the strike of the fault system (east-west direction), and $K_H = 10^{-8}$ m/sec perpendicular to this feature.

The specification of boundary conditions was based on a contoured interpretation of the measured potentiometric data[4], which indicates that no-flow boundary conditions are appropriate along the southern and eastern boundaries in the southeastern corner of the grid. Pressures were prescribed to the remaining boundary grid blocks based on a visual interpolation of these measured potentiometric data.

The Pennsylvanian-aged rocks between the upper aquifer and the Leadville were modeled as being essentially impermeable throughout the modeled region, with the exception of two areas. The relatively high potential of 1,780 m at the western end of Verdure Graben is believed to be due to downward flow from the upper aquifer into the Leadville at the intersection of Verdure Graben and the Abajo Mountains. Downward flow through this assumed avenue of high vertical conductivity results in a mound in the Leadville potentiometric surface. The mound is elliptical in shape due to the assumed anisotropic nature of Verdure Graben. The no-flow boundary condition described above coincides with the axes of this assumed elliptical potentiometric mound. Significant vertical communication between the upper aquifer and the Leadville is also believed possible in the region along the Colorado River between Dark and Gypsum Canyons (see Fig. 1). This is due to the reduced

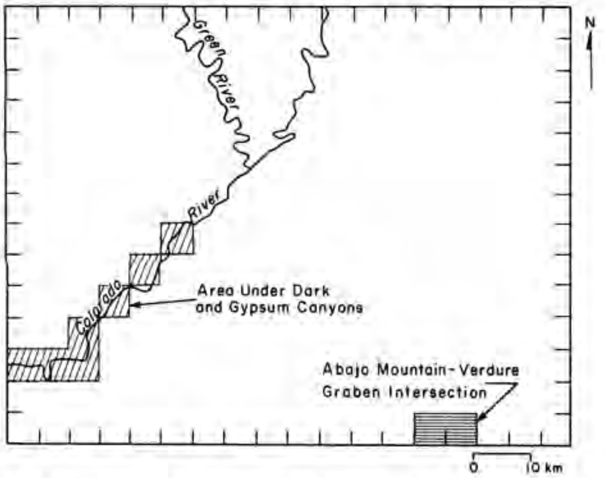

Fig. 5. Areas where vertical hydraulic communication is modeled between the upper aquifer and the Leadville.

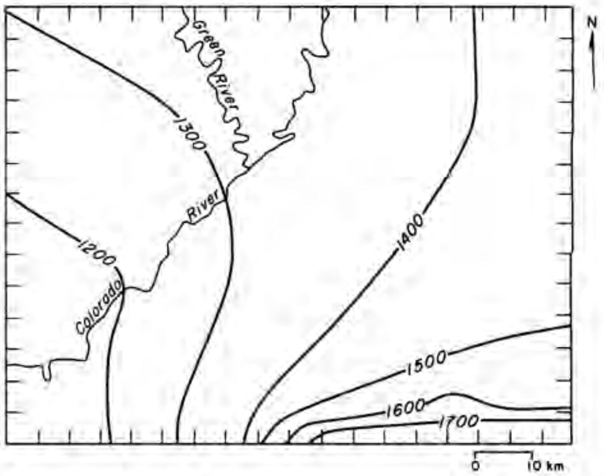

Fig. 6. Modeled Leadville potentiometric surface in meters above mean sea level.

thickness of the low permeability units between the upper aquifer and the Leadville in this region, which are as little as 60 m thick[9]. Based on the published potentiometric data[4], upward flow would occur from the Leadville to the upper aquifer in this region. A vertical hydraulic conductivity of 10^{-9} m/sec across the low conductivity units was assumed for both this region and the intersection of the Abajo Mountains and Verdure Graben, over the areas shown in Fig. 5.

The modeled Leadville potentiometric surface for this parameterization is shown in Fig. 6. Inflow to the Leadville occurs through the Abajo Mountain-Verdure Graben intersection and across prescribed pressure boundaries in the eastern half of the grid. Outflow from the Leadville occurs across prescribed pressure boundaries in the western half of the grid and upward under the Colorado River between Dark and Gypsum Canyons. Ground-water flow is directed northward to the north of Verdure Graben, northwestward near Davis Canyon and west - southwestward in the western half of the grid.

ADJOINT SENSITIVITY ANALYSIS USED TO AID IN MODEL CALIBRATION FOR THE LEADVILLE

Twenty-six of the measured potentiometric heads shown in Fig. 2 were used in the adjoint sensitivity analysis for the average squared deviation between measured and modeled pressures performance measure. These 26 measured heads are shown in Fig. 4 at the centers of the grid blocks to which they were assigned. Note that the relatively high measured head of 1,780 m located at the western end of Verdure Graben was included in the analysis. While this measured head is located to the south of the conceptual model and the kriging exercise indicated that it is an anomaly with respect to the other measured heads, there appears to be a physical basis for this head, and, in fact, the existence of this relatively high head was influential on the development of the conceptual model. As previously discussed, the head of 1,780 m is explained by vertical leakage from the upper aquifer through the intersection of Verdure Graben and Abajo Mountain and a relatively high east-west conductivity for Verdure Graben. The resulting elliptical potentiometric mound in the Leadville coincident with Verdure Graben was the basis for the no-flow boundary condition for the Leadville in the southeast corner of the grid. Thus the head of 1,780 m was included in the calibration exercise as it played a key role in the development of the conceptual model, and the modeled potentiometric surface should reflect this value.

The head of 1,134 m in Lisbon Valley (see Figs. 1 and 2) was also identified as an anomalous value by the kriging exercise. Oil and gas production occurs in Lisbon Valley, and this relatively low head is probably explained by its proximity to a production field. Oil and gas production are not included in the existing conceptual model, as the impacts of this production on ground-water flow in the Leadville are believed to be localized. Thus, this head value was not used in the calibration exercise, as it is inconsistent with the underlying assumptions used to develop this conceptualization of regional ground-water flow for Paradox Basin. If oil and gas production does in fact impact regional ground-water flow patterns in the Leadville, then the conceptual model will have to be modified before the head of 1,134 m is used in the average squared deviation between measured and modeled pressures performance measure.

The 26 measured heads from Fig. 2 that were used in the calibration exercise were converted to pressures at depth, as this is the measure of fluid potential calculated by SWENT and used in the performance measure. These 26 pressures at depth ranged from 4×10^6 to 3×10^7 Pa, and the average squared deviation between these measured pressures and the corresponding modeled pressures was 3×10^{11} Pa^2. Sensitivity coefficients were computed for this performance measure to individual grid block hydraulic conductivities and boundary conditions, and these sensitivity coefficients were summed over the geologic features identified in Figs. 4 and 5 and along the Leadville prescribed pressure boundaries. Thus, the hydraulic conductivity zones and prescribed pressure boundaries defining the major avenues of flow into, through and out of the Leadville were used in the adjoint sensitivity analysis.

Sensitivity Coefficients to Prescribed Leadville Boundary Pressures

The sensitivity coefficients of the average squared deviation performance measure to individual

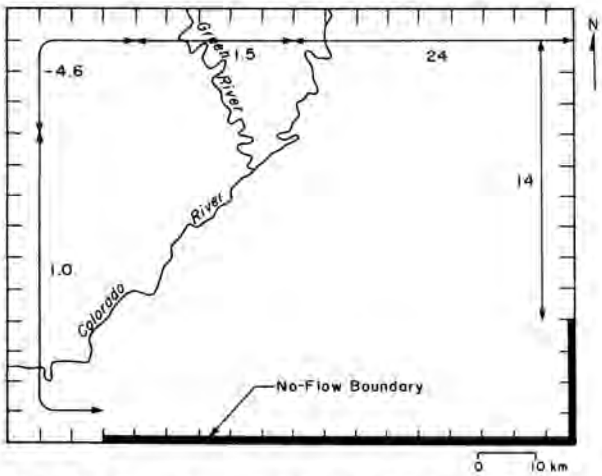

Fig. 7. Summed sensitivity coefficients for the average squared deviation between modeled and measured pressures to prescribed Leadville boundary pressures.

prescribed Leadville boundary pressures were grouped according to sign, magnitude and spatial location, and these summed sensitivity coefficients are presented graphically in Fig. 7. An improved fit between measured Leadville potentials and the modeled Leadville potentiometric surface is represented by a reduction in the average squared deviation between measured and modeled pressures performance measure. Thus prescribed boundary pressures for which positive sensitivity coefficients were calculated must be reduced in order to improve the fit of measured to modeled conditions, whereas prescribed pressures for which negative sensitivity coefficients were calculated must be increased.

As shown in Fig. 7, a 1 percent decrease in the values of all eastern prescribed boundary pressures will result in approximately a 14 percent reduction in the performance measure. The eastern boundary prescribed pressures are on the order of $2x10^7$ Pa, and thus a 1 percent reduction in these values is equivalent to a reduction of 20 m of freshwater head. Individual sensitivity coefficients on the eastern half of the northern boundary are all greater than 1, and they sum to 24, indicating that a small reduction in these prescribed boundary pressues will also have a large impact on the performance measure. It is clear from the sensitivity coefficients that the prescribed boundary pressures for the eastern half of the grid are high with respect to the measured potentials in the northeast portion of the grid. Small reductions in these prescribed boundary pressures could substantially reduce the performance measure and thus improve the fit between measured potentials and the modeled Leadville potentiometric surface.

In the northwestern corner of the grid, sensitivity coefficients of the performance measure to prescribed boundary pressures are negative for seven grid blocks, and these sensitivity coefficients sum to -4.6. This indicates that these prescribed boundary pressures are low with respect to the five measured potentials in the northwest corner of the grid, and a 1 percent increase in these prescribed boundary pressures will result in approximately a 5 percent reduction in the performance measure.

The sensitivity coefficients for the five remaining prescribed boundary pressures along the northern boundary are all positive and less than 1, and they sum to 1.5. The reduced impact of these boundary pressures on the performance measure in comparison to those discussed above is due to the fact that they are more consistent with the measured Leadville potentials, and thus smaller modifications to these prescribed boundary pressures are required in order to fit the modeled Leadville potentiometric surface to the measured potentials.

A 1 percent reduction in all prescribed boundary pressures in the southeastern corner of the grid results in only a 1 percent reduction in the performance measure. Due to the relatively large distances between these prescribed boundary pressures and the majority of the locations with measured potentials, changes in these prescribed pressures have reduced influence on the fit of modeled to measured conditions.

Note that the sensitivity coefficients are interpreted as the approximate percentage change in the value of the performance measure for a 1 percent change in prescribed boundary pressures rather than the exact percentage change in the value of the performance measure. For example, it can be stated from Fig. 7 that a 1 percent reduction in the prescribed boundary pressures on eastern boundary and the eastern half of the northern boundary results in approximately a 38 percent reduction in the performance measure. An inherent assumption to this statement is that the performance measure is linear with respect to each of the individual prescribed pressures over the ranges in pressure bracketing the existing and reduced prescribed boundary pressure values. Prescribed pressures along the eastern boundary and the eastern half of the northern boundary were reduced by 1 percent to verify this result by direct simulation. The value of the performance measure was reduced by 30 percent with the new parameterization. The reduction in the average squared deviation performance measure predicted by the adjoint method of 38 percent and the actual reduction in the performance measure of 30 percent are considered to be in good agreement, given the assumption discussed above. For the parameterization with the reduced prescribed pressures along the eastern boundary and the eastern half of the northern boundary, adjoint sensitivity results indicate that a further 1 percent decrease in these prescribed pressures will result in an additional 32 percent decrease in the performance measure. Thus a further reduction in these boundary pressures will further improve the fit of modeled to measured conditions; however, the degree of improvement is slightly less for this case.

Sensitivity Coefficients to Hydraulic Conductivity

Sensitivity coefficients for the average squared deviation between modeled and measured pressures performance measure to the hydraulic conductivity values of the geologic regions identified in Figs. 4 and 5 are provided in TABLE I. Two of the highest sensitivity coefficients are for the east-west and north-south components of hydraulic conductivity for Verdure Graben. These sensitivity coefficients indicate that an increase in Verdure Graben east-west conductivity combined with a decrease in north-south conductivity, which effectively increases the horizontal anisotropy within the fault system, will reduce the value of the performance measure. The modeled head of 1,693 m at the western end of Verdure

TABLE I

Summed Sensitivity Coefficients for the Average Squared Deviation Between Modeled and Measured Pressures to Regionalized Values of Hydraulic Conductivity

Region	Summed Sensitivity Coefficient
Verdure Graben K_H (East-West Direction)	-6.4×10^{-2}
Verdure Graben K_H (North-South Direction)	1.8×10^{-1}
Base Leadville K_H Value	2.0×10^{-1}
Monument Upwarp K_H	1.7×10^{-3}
Abajo Mountain K_H	5.3×10^{-4}
K_V Through Abajo Mountain-Verdure Graben Intersection	-5.6×10^{-2}
K_V Under Dark and Gypsum Canyons	-4.2×10^{-2}

Graben is low with respect to the measured value of 1,780 m, and the above modifications to the parameterization of Verdure Graben would reduce this differential. An increase in the vertical hydraulic conductivity of the Abajo Mountain-Verdure Graben intersection would have the same effect, as it would allow greater quantities of ground water to recharge the Leadville from the upper aquifer. The squared deviation between the modeled and measured pressures at the western end of Verdure Graben is one of the largest of the 26 squared deviations that constitute the performance measure. Thus small variations in the modeled hydraulic conductivities of these geologic features will result in a relatively large change in the performance measure in comparison to the changes that would be induced as a result of equivalent variations to modeled hydraulic conductivities for the other geologic features, even though only one pair of modeled and measured pressures is directly affected.

The largest sum of sensitivity coefficients for hydraulic conductivity zones occurs for the area assigned the base hydraulic conductivity value. The relatively large magnitude of this value is for the most part due to the number of grid blocks contributing to the sum. Based on the sensitivity coefficient, a 1 percent decrease in the base hydraulic conductivity value will result in approximately a 0.2 percent decrease in the average squared deviation performance measure. On the other hand, the small summed sensitivity coefficient for Abajo Mountain shows that the average squared deviation performance measure is relatively insensitive to the modeled hydraulic conductivity of this region. The Abajo Mountains represent a relatively impermeable feature in the Leadville, and it remains impermeable even with a 1 percent increase in hydraulic conductivity. As such, small modifications in the value of hydraulic conductivity for the Abajo Mountains will have little impact on the value of the performance measure.

Based on the adjoint sensitivity results for the average squared deviation between measured and modeled pressures, the following approach should be taken to improve the fit of the modeled potentiometric surface to the measured potentiometric data:

1. Adjust the prescribed boundary pressures, particularly those along the eastern boundary and the eastern half of the northern boundary, as the sensitivity coefficients indicate that the Leadville prescribed boundary pressures (Fig. 7) have a greater impact on the average *squared* deviation performance measure than hydraulic conductivities (TABLE I).
2. Recompute adjoint sensitivity coefficients for this performance measure to the regionalized values of hydraulic conductivity using the adjusted prescribed Leadville boundary pressures, and where appropriate adjust these hydraulic conductivity values within their ranges of uncertainty to further improve the fit of the modeled potentiometric surface to the measured potentiometric data.

DISCUSSION

The application of geostatistical and adjoint sensitivity techniques in the calibration of an existing conceptual model of ground-water flow to measured potentiometric data was demonstrated. The geostatistical method called kriging was used to characterize the correlation structure between the measured potentiometric data. Additionally, two anomalous potentiometric data were identified. Physical explanations were suggested for both of these potentiometric heads, and as a result one value was removed from the data set. Adjoint sensitivity analysis was then used to aid in the calibration of the existing conceptual model of ground-water flow to this reduced set of measured potentiometric data. Sensitivity derivatives calculated by the adjoint method were used to identify model parameters and boundary conditions that had the most influence on the fit of modeled to measured potentiometric conditions, and a strategy for model calibration was presented.

The kriging and adjoint sensitivity techniques can be better integrated to more effectively develop a conceptual model of ground-water flow that is calibrated to measured potentiometric data. This is illustrated by the large sensitivity coefficients for the fit between modeled and measured potentiometric conditions to prescribed boundary pressures. The practice of visually interpolating prescribed boundary potentials from measured potentiometric data, as was done in the development of the existing conceptual model, does not always result in a satisfactory representation of observed flow conditions. Instead of visually interpolating prescribed boundary potentials, the semi-variogram that was developed by the kriging technique can be used in combination with the measured potentiometric data to statistically estimate potentiometric heads for prescribed-boundary grid blocks and the uncertainties in those values. The estimated potentiometric heads would be used to calculate prescribed boundary pressures, and the estimated uncertainties would provide an indication of the extent to which the prescribed boundary pressures could be varied in order to improve the fit of the modeled potentiometric surface to the measured potentiometric data.

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