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Flow Model Development for the Idaho National Laboratory OU 10-08 Sitewide Groundwater Model

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ABSTRACT

A two-dimensional (2D), steady-state groundwater flow model was developed for the Idaho National Laboratory (INL) sitewide groundwater model. A total of 224 wells inside the model domain were used to calibrate the 2D flow model. Three different calibration techniques, zonation approach, pilot point approach and coupled zonation/pilot point approach, were explored and applied during the model development. The pilot point approach allows modelers to model aquifer heterogeneities at various scales, and extract the maximum amount of data from available monitoring data, permitting the best possible representation of flow and transport at the INL.

INTRODUCTION

During fiscal year 2005, a two-dimensional (2D), steady-state INL sitewide groundwater flow model was constructed for Operable Unit 10-08. The 2D steady-state model provided an intermediate step in the development of a fully three-dimensional numerical tool that can evaluate cumulative risk of INL-derived contaminants in groundwater.

Comment [MSOffice1]: This text will help to explain overall modeling objective.

DEVELOPMENT OF THE 2D FLOW MODEL

The computer codes used to develop the 2D flow model were the MODFLOW-2000 (Harbaugh et al. 2000) groundwater flow simulation code, the PEST (Doherty 2005) parameter estimator, and the Groundwater Modeling System (GMS) (BYU 2003) pre- and post-processor and data analyzer. The following subsections summarize the implementation of the conceptual model into a 2D steady-state numerical flow model using GMS/MODFLOW-2000/PEST.

Model domain/boundary conditions and calibration wells.

Figure 1a shows the model domain implemented in the 2D flow model. The northern and southern boundaries of the OU 10-08 model domain are treated as specified head boundaries. The eastern boundary of the model domain extends in a northeast-to southwest direction and corresponds to an estimated groundwater flowline across which there is no groundwater flow. The model domain is bounded on the west by a Type 2 boundary (part no-flow and part specified-flux) that represents mountain ranges and the mouths of significant tributary streams. Head values along these two specified head boundaries are derived from the June 2004 water table map. The major sources to the flow model include infiltration recharge from the Big Lost River and precipitation recharge, underflow from the northeastern boundary and underflow from the adjacent tributary drainage basins to the northwest (see Orr et al. 2006, this issue). Figure 1a also shows the locations of all 224 wells that provided head measurements used in the calibration. At the current stage of model development, all head measurements at these 224 wells have been assigned equal weights.

Construction of the 2D numerical grid

Figure 1b shows the model grid of the 2D flow model, a single layer with variable thickness derived by the conceptual model (see Orr et al. 2006, in this volume). The grid shown here corresponds to a “thin” aquifer thickness scenario. The grid is refined near facilities inside the INL in order to capture some important local-scale features. The grid cell dimensions have a minimum size of 492 ft (150 m) near nine individual WAGs, and maximum size of 2,460 ft (750 m) elsewhere inside the model domain. Such discretization results in a total of 53,658 grid cells.

Calibration approaches

Three calibration techniques, zonation, pilot point and coupled zonation/pilot point, have been tested in the development of the 2D flow model. All three calibration techniques were implemented with PEST ((Doherty 2005), an automated parameter estimator.

The zonation approach is a traditional method of calibration. This approach divides the model domain into zones of constant hydraulic conductivity, then adjusts the hydraulic conductivity values to minimize the mismatch between the model simulated and measured heads at all calibration wells.

The pilot point approach is a more numerically advanced inverse modeling technique. Instead of dividing the model domain into a number of zones, a number of “pilot” points are positioned within the model domain, then hydraulic conductivities at these pilot points are adjusted to minimize the mismatch between model simulated and measured heads. The hydraulic conductivities of each model grid cell are interpolated from the conductivity values at all pilot points.

The coupled zonation/pilot point approach takes advantage of both approaches. In this coupled approach, the model domain is first divided into different zones. Then within each zone, a set of pilot points is distributed, resulting in the capability for the hydraulic conductivity to vary within each zone. The coupled pilot-point/zonation approach provides a good combination of the large-scale heterogeneity (from zone to zone) and local-scale heterogeneity (inside a zone).

Calibration results

Table 1 summarizes residual statistics between the measured and model simulated heads in the OU 10-08 model domain obtained by the three calibration approaches. As shown in Table 1, the zonation approach provides the worst fit to the measured heads, while the coupled approach provides the best fit. The pilot point approach also provided a good fit to the measured heads, compared with the zonation approach. However, simply comparing residual statistics alone is misleading for evaluating the calibration results. We also have evaluated the reliability of the estimated parameters.

The first step in evaluating the reliability of the estimated parameters is to compare the parameter field with the known features. Figure 2 shows the comparison of the hydraulic conductivity fields obtained by three calibration approaches. The most significant result from this comparison is that the pilot point approach provides the conductivity field most consistent with the known large-scale geological features inside the model domain (Helm-Clark, 2006, this issue).

A more quantitative way to evaluate the reliability of the estimated parameter field is to examine the confidence bounds associated with each estimated parameter. Large confidence bounds are strong indicators that the estimated field is highly uncertain. Figure 3 shows the confidence intervals of the estimated hydraulic conductivities by the three calibration approaches. Both the zonation approach and the coupled approach exhibit very large confidence bounds of several orders of magnitude difference between the upper and lower bounds, indicating that the estimated conductivity fields by these two approaches are highly uncertain. However, the confidence bounds for pilot point approach are much narrower, and most bounds are less than 1 order of magnitude, indicating the parameter field estimated by this approach provides a much more reliable representation of heads.

SUMMARY

The objective of developing the current 2D flow model is to better understand both the regional and local-scale features, investigate the validity of various calibration approaches, and investigate the feasibility of using all available wells as calibration wells as an intermediate step in development of a fully three-dimensional numerical tool. Although the 2D modeling results (primarily the pilot-point approach) have proved to be satisfactory in terms of meeting the above objective, this 2D model has some important limitations, particularly in the area of accurately addressing the contaminant transport problems.

Although we have used variable thickness, the 2D model assumes the hydraulic conductivity and head are the same along the vertical direction. So the estimated hydraulic conductivity field and simulated head are the averages across the entire aquifer thickness. However, there is strong evidence that the vertical heterogeneity of the aquifer could control potential vertical flow within the system. This feature likely will have important impacts on contaminant transport predictions.

Another limitation of the 2D model is its inability to reproduce the “preferential” flow path identified through geochemical and isotope studies in the INL Site. This preferential flow path again may have an important impact on the transport of contaminants. One hypothesis is that the preferential flow path might be a feature occurring only within the upper portion of the aquifer, while the 2D model can only address the lumped (averaged) effect across the entire thickness of the aquifer. Only a three-dimensional model can incorporate such vertical heterogeneity. If the preferential flow path does exist, it will lead to much faster contaminant transport than we expected, and a three-dimensional model is required to test this hypothesis.

Evidence presented elsewhere (Whitmore, et al, 2006 and Roddy, 2006, this issue) indicates that contaminants are preferentially transported in the upper portion of the aquifer and in narrow flow pathways. However, the two-dimensional model is capable only of the assumption of uniform concentrations across the entire thickness of the aquifer. Thus, contaminant flux entering the aquifer immediately mixes (or dilutes) in the vertical direction across the full thickness of the aquifer. This leads to an unrealistic underestimate of contaminant concentrations in the 2D model.

Comment [MSOffice2]: Actually, the narrow flow pathways discussion is presented by McLing and Roback.

Due to the limitations of the 2D flow model, we conclude that a fully three dimensional model that incorporates both horizontal and vertical heterogeneities at various scales is required to accurately depict and predict the contaminant transport in the SRPA.

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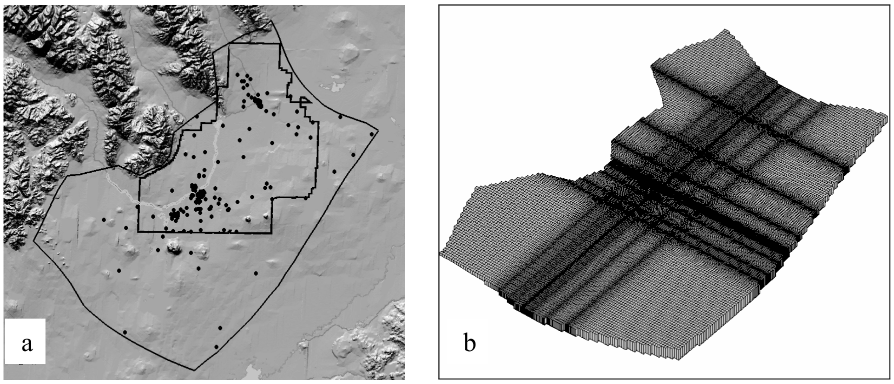
Table 1. Statistics of the residuals (in meters) between measured and model simulated heads.

	Zonation	Pilot point	Coupled zonation/pilot point
Mean Error	0.240	-0.246	0.054
Mean Abs. Error	1.521	0.488	0.273
Root Mean Sq. Error	3.069	0.684	0.413



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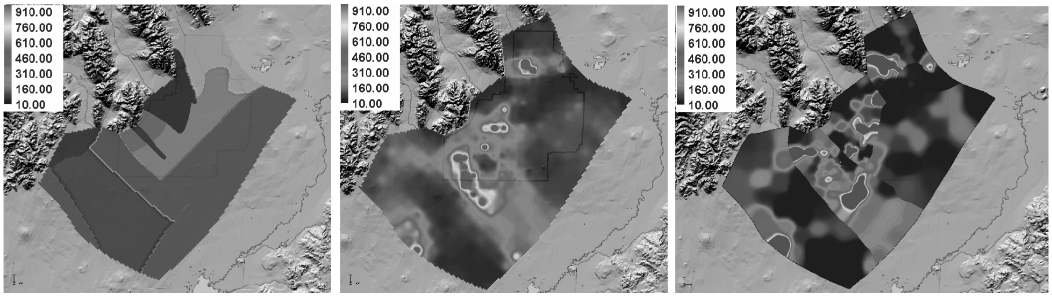

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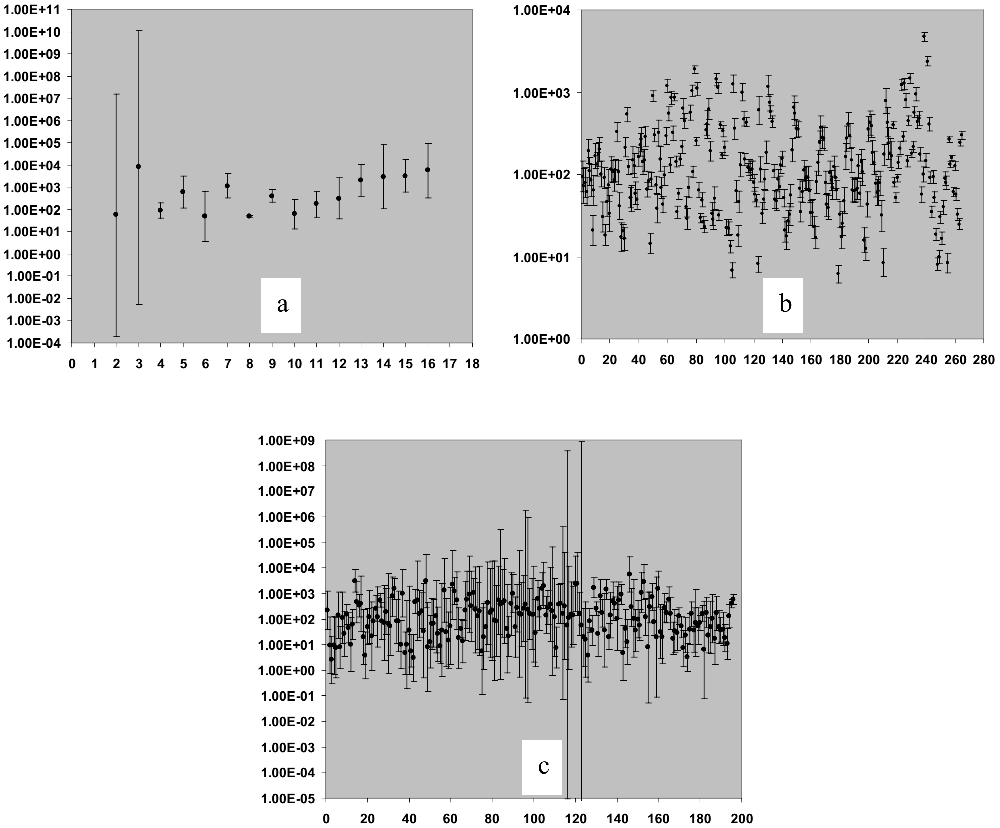

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