

Interactive comment on “Bayesian approach for three-dimensional aquifer characterization at the hanford 300 area” by H. Murakami et al.

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We appreciate the constructive comments. The responses to the comments are as follows. One figure (Fig. C2-1) was added at the end of this document.

Response to Comment Number 3:

We will expand the conclusion section by adding discussion about (1) the difference between MAD and other inverse modeling methods and (2) the contribution of this paper to groundwater modeling. The details are provided in the responses below.

C2175

Response to Comment Number 4(1):

Rubin et al. (2010), now in press and available on the website of Water Resources Research, goes into substantial detail in comparing MAD to other inverse modeling methods. The major advantages of MAD are the following:

- (1) MAD is directly connected to stochastic modeling of groundwater flow and transport, since it can directly infer the joint distribution of the parameters to be used as an input for stochastic simulations.
- (2) MAD fully quantifies the parametric uncertainty as the statistical distribution.
- (3) MAD does not incur overfitting problems, since it uses neither fitting nor optimization procedures.
- (4) Given its modular structure, MAD is not limited to any type of data or model, which opens the door for applications with a wide variety of data types and modeling tools.

Response to Comment Number 4(2):

In the stochastic simulations, each of the simulated results is a possible outcome conditioned on the data. The way we chose to evaluate the inversion results was by comparing predictions with the testing set data, i.e., the observations not included in the inversion. It is a common procedure in statistics to divide the dataset into a training set (i.e., data used in inversion) and testing set (i.e., data used for testing or validating the inversion result). Figure 8 shows that the prediction captures the actual observations, and increasing the number of observations makes the distribution tighter around the actual values.

We would like to add that the large number of realizations does not eliminate uncertainty; it leads to more reliable predictions. Some uncertainty is irreducible (e.g., due to measurement errors or data scarcity)

C2176

Response to Comment Number 4(3):

We added several realizations of the 2-D $\ln T$ field for the transect, which are the actual fields to be used for stochastic simulations of flow and transport. Please see Response to Specific Comments Number 5 by Anonymous Referee #1.

Response to Comment Number 4(4):

We gradually added more simulations until we observed the posterior distribution remaining the same, i.e., not changing along with further increasing numbers of simulations. Increasing the number of simulations does not narrow down the distribution, but rather leads to a more accurate representation of uncertainty. So in general, there should not be the expectation that an increasing number of simulations should lead to deterministic convergence. Regarding increasing the number of injection tests, please see Responses to Specific Comment Number 4 by Anonymous Referee #1.

Response to Comment Number 4(4) "This is related to my comment 3 above. I think it would be better that the authors add some discussion about the results from the perspective of groundwater modeling.":

Regarding the perspective of groundwater modeling, we will expand the discussion in the conclusion section to address this concern, including:

(1) The aquifer in the Hanford formation has been very difficult to characterize due to the coarse-grained and highly permeable nature of the aquifer, since typical methods, such as permeameter tests and slug tests, do not provide reliable results. In addition, pumping and injection tests yield only the averaged property over a large domain, since

C2177

the zone-of-influence expands very rapidly, as we discussed in Section 2 of the paper. In this paper, we have shown that the combination of the EBF and injection tests is promising for characterizing the heterogeneous $\ln K$ field in such an aquifer.

(2) The 3-D characterization is restricted by the EBF measurement density, in the sense that increasing depth-averaged information from the injection tests did not contribute significantly to narrowing down the posterior distribution of the 3-D geostatistical parameters. This finding is consistent with Li et al. (2008).

Response to Comment Number 4(4) "When posting my comment, I read the comment of Dr. Zhang. I guess he might be right about the dimensionality of the likelihood. But I am not entirely sure since the largest parameter dimension that I worked on is 8 and my MCMC simulations gave satisfactory results.":

Regarding Dr. Zhang's concern, we used a parametric approach for the likelihood estimation in this paper. We confirmed that the number of realizations per parameter set was sufficient, in the sense that the likelihood values did not change any further with increasing numbers of realizations.

Figure C2-1 shows the change in the estimated likelihood with increasing numbers of realizations, compared to the one based on 250 realizations. We used the injection test at Well 2-09, which has the most observation wells. Since the likelihood computed from 230 realizations is not different from the one computed from 250 realizations, we may consider that 230-250 realizations are sufficient for the likelihood estimation. We therefore used 250 realizations for our inversion.

In terms of the parameter dimension, although our parameter vector, including three structural parameters and 44 anchors, has 47 dimensions, some of the parameters are strongly correlated (e.g., adjacent anchors), which leads to fewer parameter sets required for convergence than a independent-parameter case. Fu and Gomez-

C2178

Hernandez (2009), for example, applied the Bayesian inference for hydrogeological inverse modeling, considering all the 32-by-32 grid points in the parameter vector (1024-dimensional parameter vector). They reported that they obtained convergence with 10^3 - 10^5 parameter sets. From this reference, it would be reasonable that the number of parameter sets we used (i.e., 36,000 parameter sets) was more than sufficient for the 47-dimensional parameter vector.

Response to Comment Number 6:

The forward simulations for nine million realizations (4 tests) took a total 10 hours using 9,000 cores on the Franklin supercomputer at the National Energy Research Scientific Computing Center (<http://www.nersc.gov/>). The post-processing, including the likelihood estimation, took less than thirty minutes for all cases on our desktop computer (Intel Core 2, 3GHz). Since the high-performance computing (HPC) facilities have recently become more readily available for researchers throughout the world, we consider that the amount of time and computer resources expended was reasonable.

Response to Comment Number 8:

While we used MAD for the 2-D pumping test injection, we used Bayesian model-based geostatistics for inferring the structural parameters of the 3-D $\ln K$ field. We consider the general name to be appropriate.

C2179

Response to Comment Number 11(1):

Corrected.

Response to Comment Number 11(2):

Corrected.

Response to Comment Number 12(1):

Y is a random variable at a location \mathbf{x} . The field is a collection of Y , which is a random vector denoted by \tilde{Y} . (We will modify the paragraph to avoid confusion.)

Response to Comment Number 12(2):

We will expand the explanation in the paper. The vector \mathbf{z} is the measured outcome, whereas $\tilde{\mathbf{z}}$ is one realization. By generating random fields for a given parameter set $\{\vartheta, \theta\}$ and simulating injection tests on each field, we obtain multiple realizations of $\tilde{\mathbf{z}}$, i.e., an ensemble of $\tilde{\mathbf{z}}$. Since we assume that the probability density function (pdf) of $\tilde{\mathbf{z}}$ is multivariate Gaussian, estimating the pdf is equivalent to calculating the mean and covariance of the ensemble. The measurement error variance is added to the diagonal elements of the covariance, since the measurement errors are independent. After determining the pdf, it is straightforward to calculate the density at a point \mathbf{z} , $p(\mathbf{z} | \vartheta, \theta)$, which is the likelihood.

C2180

Response to Comment Number 12(3):

It is true that increasing the number of observations within one test does not add computation for one realization. However, when the dimension of \mathbf{z} increases, a larger number of realizations of \mathbf{z} are necessary to estimate the pdf accurately. We will revise the text to avoid the confusion.

Response to Comment Number 12(4):

In Page 2026 (Line 18), $\mathbf{R}(\mathbf{x}, \mathbf{x}_\vartheta)$ is defined as the cross-correlation matrix between \mathbf{Y} and ϑ . Since theta is the structural parameter vector, it does not have locations. In the paper, all the subscripts for \mathbf{x}_ϑ are vartheta ϑ .

Response to Comment Number 12(5):

We gradually increased the number of realizations of anchor values until increasing the number of realizations did not change the posterior distribution. The same set of anchors is used for all the simulations.

Response to Comment Number 12(6):

Following Li et al. (2008) and Nowak et al. (2005), we included measurement errors based on fluctuation or noise in the measurements, which is the instrument resolution in our case. We multiplied it by the observation time, since the zeroth-order moment at each well is an integral of the pressure buildup curve. This measurement error is

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honored in the likelihood estimation, as is described in Response to Comment Number 12(2).

Additional References

Fu, J. and Gómez-Hernández, J.J: A blocking Markov Chain Monte Carlo method for inverse stochastic hydrogeological modeling, *Math. Geol.*, 41(2), 105–128, 2009.

Complete Figure Captions

* Due to the limited space, caption below the figure was truncated.

Figure C2-1. Estimated likelihoods (L.) $p(\mathbf{z}_1 | \vartheta, \theta)$ for the first 9,000 parameter sets $\{\vartheta, \theta\}$ out of 36,000 sets randomly generated in the inversion, based on different numbers of realizations, compared to the one based on 250 realizations; (a) 50, (b) 100, (c) 150, (d) 200, (e) 230 and (f) 240 realizations. The sum of likelihoods in each case is normalized to one. The red line is the one-to-one match line.

Interactive comment on *Hydrol. Earth Syst. Sci. Discuss.*, 7, 2017, 2010.

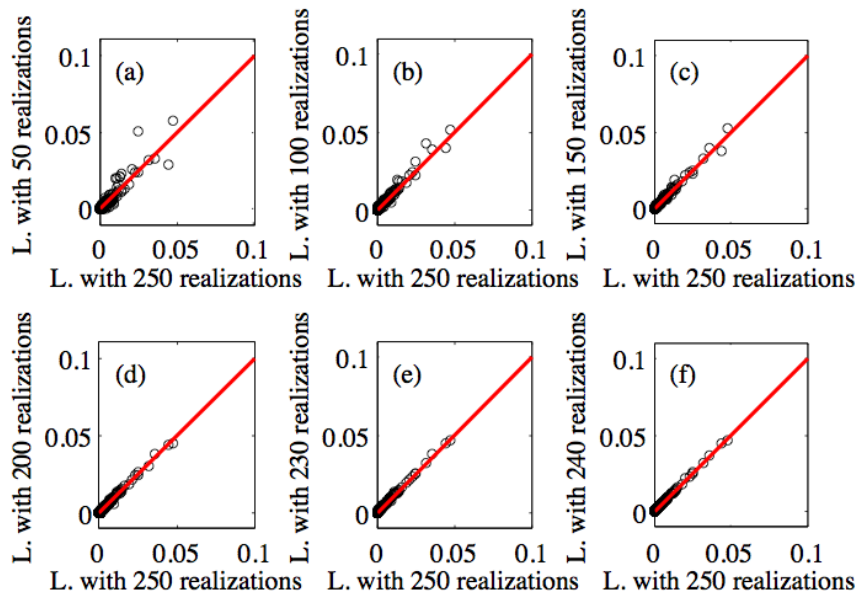


Fig. 1. (Figure C2-1). Estimated likelihoods L_i for the first 9,000 parameter sets θ out of 3