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

Anonymous Referee #2

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This paper presents an evaluation and application of a recently developed method, Method of Anchored Distributions (MAD), using a (semi-)synthetic and a real-world case at the Hanford Site of the U.S. Department of Energy (DOE). Overall, this is a well written manuscript, and it certainly should be of interest to colleagues working on hydrologic inverse modeling. Below are my comments that may be useful to the authors.

1. Does the paper address relevant scientific questions within the scope of HESS?
Yes. I believe that groundwater inverse modeling is a relevant scientific question within the scope of HESS.

2. Does the paper present novel concepts, ideas, tools, or data?
This paper is focused mainly on evaluation and application of MAD, not on developing new concepts and ideas. Nevertheless, in my point of view, this paper indeed demonstrates that MAD is a useful tool for groundwater inverse modeling.

3. Are substantial conclusions reached?
The conclusions are a little weak. If I am not mistaken, there are essentially only two major conclusions: (1) MAD gives satisfactory results in the synthetic case, and (2) application of MAD at the Hanford Site is feasible and the results are acceptable. While these two conclusions warrant publication of this paper (regarded as a numerical experiment) at HESS, I think there are more issues (both numerical and hydrogeological) that the authors can explore based on the numerical results. Some examples are given in my comment below.

4. Are the scientific methods and assumptions valid and clearly outlined?
I am not entirely clear myself what a good groundwater inverse method should be. Some intuitive thoughts relevant to MAD are as follows:

(1) MAD should be competitive to, if not better than, other inverse methods. Since this is a numerical study, it should be relatively easy to compare the calibration results of MAD with those of other methods such as the least square method (LS). Such comparison is not shown in the paper. Although the comparison may not be very meaningful because MAD is Bayesian and LS is deterministic, a comparison would be of interest to the community.

(2) MAD should provide acceptable (defined by modelers subjectively) goodness-of-fit to observations. Although the goodness-of-fit is always measured by statistics such as mean square error, I think a direct comparison between observations and corresponding simulations are necessary, because it reveal more direct information of the goodness-of-fit. This can be easily done for deterministic calibration such as the least...
square or maximum likelihood methods, but it is no very straightforward for stochastic calibration such as the Bayesian method of MAD, because its simulations are probabilistic. In this paper, the goodness-of-fit is discussed for the real-world modeling in Figure 8, but not for the synthetic case. This may be OK, since Figure 6 shows that the true parameter fields are included in the 98% confidence intervals. However, I am wondering what the variance of the predicted zeroth-order moment is. Since 9,000,000 realizations are used in the calibration, I would expect that the variance is very small.

(3) For the synthetic study in which the true groundwater model is known, one would expect that the calibrated parameter fields of MAD are close to the true field; otherwise, the calibration method is problematic. While this comparison is not straightforward for the Bayesian method of MAD, showing several parameter fields would be useful. I am particularly interested in the field generated using the mean structure parameters given in Figure 5 and associated anchors. It is anticipated that this field is close to the reference field plotted in Figure 4. For real-world modeling, the calibrated parameter fields are not very important, because the numerical model used as the basis of model calibration is an approximation of reality. One cannot expect that the calibrated parameters of the approximating model can reflect the reality.

(4) The calibration should help us better understand the hydrologic problem so that, for example, we know how to improve the model(s) and where and when to collect more data. I am not sure how useful MAD is in this sense. The parameter distribution is certainly useful, but I am concerned that the parameter distributions (e.g., Figures 5 and 7) are still wide for 9,000,000 simulations. What is the reason? Is it related to the anchors? On the other hand, are the 9,000,000 simulations really needed? Can convergence of the posterior distribution be achieved with less number of simulations? It is also noted that in Figure the distribution of scale of 4 tests is even more biased than that of 3 tests. What is the difference between the 3 tests and 4 tests? What would happen if all the 12 tests were used in the inverse modeling?

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.

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.

5. Are the results sufficient to support the interpretations and conclusions?
I believe so except for the comment above.

6. Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)?
The large number of simulations would hinder reproduction. The computational cost would also hinder application of MAD, in particular when nonparametric methods are used for estimating the likelihood function.

7. Do the authors give proper credit to related work and clearly indicate their own new/original contribution?
Yes.

8. Does the title clearly reflect the contents of the paper?
The title of “Bayesian approach” is too general. “Application of MAD for …” would reflect more clearly the contents of the paper.

9. Does the abstract provide a concise and complete summary?
I believe so.

10. Is the overall presentation well structured and clear?
Yes. This is a well-organized and well-written paper.

11. Is the language fluent and precise?
Yes. This is a well-organized and well-written paper. A few minor comments:

(1) In page 2020, Li et al. (2004) should be Li et al. (2005), and Zhu and Yeh (2005) be (2006).

(2) In page 2022, it would be better to point out that the parameter ranges of Meyer et al. (2007) are based on inverse modeling.

12. Are mathematical formulae, symbols, abbreviations, and units correctly defined and used?

A few minor comments:

(1) Line 8 of page 2024. What does the “entire field of Y” mean? Is it the entire ensemble of Y?

(2) Line 10 of page 2025. Since z is just one realization of z_tilt, how to estimate the likelihood p(z|theta, theta) using z_tilt? By using the distribution of the measurement error in equation (1)?

(3) Line 11 of page 2025. This sentence is a little misleading. I understand that the authors mean that z represents different tests. Simulating more tests is certainly more time-consuming. However, this sentence implies that it is the case for adding any number observations z, for example, increasing the number of observations from 10 to 100. This is not the case, since simulating 10 or 100 observations requires solving governing equation just once, if the model is of steady state.

(4) Line 18 of page 2026. R(x,x_theta) is not defined.

(5) Line 13 of page 2030. Based on what the number (12) of sets of anchors are determined? Are the same anchors used for all the simulations with different numbers of tests?

(6) Is there any uncertainty associated with estimating the zeroth-order moments? If so, how is (or would be) the uncertainty addressed in MAD?

13. Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated?

No.

14. Are the number and quality of references appropriate?

Yes.

15. Is the amount and quality of supplementary material appropriate?

There is no supplementary material.