## Reviewer #2

The comments of Jasper Vrugt are in italics

The paper is well written and addresses an important topic in hydrologic systems analysis, namely robust model evaluation. The authors draw inspiration from the Kalman Filter and bring linear algebra, Tikhonov-regularized inversion and surrogate modeling to bear to decompose and/or approximate the forward model and quantify its prediction uncertainty using relatively few model simulations. This is yet another addition to the methods of the PEST toolbox designed to enable as thoroughly as possible the uncertainty quantification of highly parameterized and CPU-demanding surface-subsurface hydrologic models for which existing Monte Carlo simulation methods are too demanding and/or cumbersome to implement. One can only applaud the efforts of the authors, particularly the 2<sup>nd</sup> author, John Doherty, to provide workable solutions (with sufficient theoretical rigor) to practical, real-world, problems.

I do not have comments on the methodology. The assumptions are almost always listed and/or defined, and the mathematics (linear algebra) articulates the implementation. I only have one comment, which I think could help to further strengthen this paper.

Thank you very much for your kind words on our approach and our work in general. As reviewer 1, no methodological issues were identified.

The present case study is well chosen to illustrate the DSI methodology. But this case study is not easy to immediately repeat. I think the authors should consider including a relatively simple hydrologic modeling study which (a) is easy to reproduce and (b) most readers are familiar with. I believe that this may help articulate the detailed workings of the presented DSI methodology.

Thank you for your comment. While reviewer 1 suggests to implement a "real" case study you suggest to rather implement a much simpler model, so the suggestions are contrary. For the following reasons we feel that our model is the sweetspot to effectively demonstrate our approach:

- The model is actually easy to reproduce and straightforward to implement. All boundary conditions are clearly described, the grid is easy to reproduce with the information provided in the paper. In any case, the input files are all provided, and can readily be used.
- We believe that the setting we are simulating is probably one of the most common settings in hydrogeology: A well next to a stream. We do not see the benefit of having a simpler model. The model has to be tailored to provide a solid basis for verification and to demonstrate the usefulness of the approach.

## *This case study does not have to be a distributed and/or computationally demanding modeling problem.*

One of the most important features of our approach is that it is capable of dealing with slow, and computationally very demanding models. We do not think that using a computationally non-demanding model is useful to demonstrate this feature.

An additional advantage of such a simple study is that the uncertainty of the DSI methodology can be benchmarked against Bayesian methods using a full exploration of the model's parameter space using MCMC simulation with/without the use of advanced distribution-free likelihood functions. This will readers to better understand the strengths and weaknesses of the presented methodology.

We do not see MCMC simulation directly comparable to DSI. DSI is independent of the number of model parameters, while the efficiency of MCMC is dependant the number of parameters employed. We understand the point of verifying the methods against a more traditional method. This work has already been done by Sun and Durlofsky (2017), who compare the results of DSI with the rejection sampling procedure. We preferred to compare our DSI procedure against the Iterative Ensemble Smoother, which is a well established method that can be used with complex models and highly parameterised environments. This is the closest approach to DSI, and therefore suitable for a benchmark comparison.

As mentioned above, to some extent our work continues that of Sun and Durlofsky (2017). This continuation embodies use of the DSI surrogate model in conjunction with linear analysis tools that support data worth analysis at very little cost. The worth of data is judged by its ability to reduce the uncertainties of model predictions of interest. To be sure, linear analysis is approximate. Its strength, however, is that it does not require that values be assigned to posited observations, nor to the parameters that they may inform. Furthermore, it can be undertaken extremely quickly once a sensitivity matrix is available. We see demonstration of this methodology using the DSI model as an important component of our paper. However, we see a comparison of the results of this analysis with MCMC (which is unable to handle enough parameters to characterise the heterogeneity of aquifers, and for which data worth assessment would need to be nonlinear) as well beyond the scope of our paper. This is especially the case where uncertainty is dominated by parameter nonuniqueness – a context in which the numerical cost of MCMC can be very high indeed. (As we point out in our paper, comparison with IES – a method that IS able to accommodate parameter nonuniqueness - was a numerically costly exercise.)

## One may interpret this as a moderate revision but at the same time, I also understand if authors wish to publish their work as is.

We thank the reviewer that he is not objecting to publication as it is. While reviewer 1 suggests a more complex model for a real case, reviewer 2 suggests a simpler model. For the reasons we outlined above, we believe that our choice of model is the most appropriate one in terms of demonstrating the capability of our approach. It is easy to reproduce, provides all the information required to assess the robustness of our approach, corresponds to a very common hydrogeological setting and allows to demonstrate the very high performance of the proposed methodology.

Best,

H. Delottier, P. Brunner and J. Doherty