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Title:

Estimating Geostatistical Parameters and Spatially-Variable Hydraulic Conductivity within a Catchment System using an Ensemble Smoother

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The reviewers’ comments have been addressed in the following sections.

Comments from Reviewer #1 (Anonymous)

General: This paper is interesting and presents a contribution for data assimilation in a surface-subsurface flow system. Not only states, but also parameters and meta-parameters (geostatistical parameters) are updated. The paper is in general well written and the contribution is novel. There are, however, some weak points of the study, in my opinion. One is that river discharge is included in the state vector, whereas it should have been assimilated as observation, and the states should have been updated through a linearized relation between states and discharge flux. I believe that that would be the more correct way to proceed. Further comments follow below. I think that the paper can be published after revisions have been made.
Authors' response: the comment on the use of streamflow as a state variable has been addressed below in our specific response to Comment 4.

Comment 1: Page 9592, Line 3. EnKF instead of EnFK.
Authors' response: On page 9592, Line 3 (discussion paper) in Section 1.2, "EnFK" has been changed to "EnKF"

Comment 2: Page 9594, L 2-5. This is a limitation of this work, as correlation scale has the highest impact on weighting in the EnKF (more than sill, for example). As other scientists had problems to estimate the correlation scale, I can imagine that the authors also tried this and were not successful here. It would be good to indicate this in the paper and provide further details on possible attempts the authors made to estimate the correlation scale.
Authors' response: The reviewer has raised an important point. When the iterative approach was first used to estimate geostatistical parameters, it became evident that the correlation scale could not be estimated with the assimilation of water table elevation data. There were no further attempts to estimate the correlation scale. The text has been revised to reflect this, and is indicated at the end of Section 2.5. It reads: "*It should be noted that estimation of the correlation scale λ was not pursued extensively in this study, as it became evident during initial uses of the iterative approach that λ could not be estimated using only a model-response variable such as water table elevation. As discussed in Section 4, the direct assimilation of Y_K values are likely required to provide information regarding λ, and will be pursued in future work.*" We hypothesize that the correlation scale may be able to be estimated if values of hydraulic conductivity are directly assimilated into the model ensemble results, but this has not yet been attempted. This hypothesis, and the intention to pursue the topic in future studies, is indicated at the end of Section 1.4, at the end of Section 2.5, and at the end of Section 4:

- *Section 1.4: "Uncertainty in correlation scales is not addressed in this study, but is left to future work. Assessment of the true correlation scale for a given aquifer will likely require the direct assimilation of K measurements, whereas in this study only the model response variables are assimilated."*
- *Section 2.5: "As discussed in Section 4, the direct assimilation of Y_K values are likely required to provide information regarding λ, and will be pursued in future work."*
- *Section 4: "For the present study uncertainty in the correlation length of the K field is not investigated, and an amendment to the iterative scheme to converge upon unknown correlation length is left to future research, with assimilation of measurements of K likely necessary."*

Comment 3: Page 9595, L 7-8. This seems not the most appropriate reference for the groundwater flow equation.

Authors' response: This is the groundwater flow equation employed by the authors of the CATHY model, which is the numerical model used in the study, and hence we feel that it is the most appropriate reference for the groundwater flow equation in this study. We therefore have not revised the text.

Comment 4: Page 9596, L 13. This is not a state, but a flux, and should therefore not be included in the state vector. Instead, a relation between the flux and state variable should be derived (using a linearization for example). Details on how to assimilate observed discharge data can for example be found in Pauwels and De Lannoy (2009, WRR). It is true that also in other papers discharge was included in the state vector, but this is not correct in my opinion.

Authors' response: We cordially disagree with the reviewer regarding this comment. The streamflow Q is a state variable solved for directly by CATHY (see Equation 2b in the paper), and thus we have included it in the state vector as a state variable without any modification. This is the standard procedure for studies using CATHY. See Camporese et al (2009, WRR) and Camporese et al. (2010, WRR).

Comment 5: Page 9601, L 24. "updated" instead of "update".

Authors' response: On page 9601, line 24 (discussion paper) in Section 2.5, "update" has been changed to "updated".

Comment 6: Page 9603, L 5. What about ET? It seems the authors applied net infiltration instead of precipitation. This should be clarified.

Authors' response: The reviewer is correct. Net infiltration was used rather than precipitation. This has been clarified in a number of locations in the paper:

- Section 3.1, paragraph 3: "*Forcing terms q_{ss} consist of uniformly-distributed net infiltration from precipitation during the months of January through March and November through December, and spatially-varying rates of net infiltration from applied water (e.g., irrigation water) in addition to net infiltration from precipitation during the months of April through October.*"
- Section 3.1, paragraph 3: "*As an example, the rates of net infiltration from combined precipitation and applied water for the month of July for one realization are shown in Figure 4B, with values ranging from 0.000355 m day^{-1} to 0.006 m day^{-1} (represented by white and black, respectively). The depth of monthly net infiltration is presented in Figure 2.*"
- Section 3.1, paragraph 4: "*The streamflow rate at the outlet cell of the catchment is shown in Figure 5B, indicating the increased discharge during the months of April through October due to increased rates of net infiltration from precipitation as well as applied water.*"
- Figure 2 has also been modified to include the axis title "Net Infiltr. from Precip." rather than "Precipitation" on the inset graph.

Comment 7: Page 9603, L 17. Change to: "an isotropic, homogeneous aquifer."

Authors' response: On Page 9603, line 17 (discussion paper) in Section 3.1., "and isotropic, homogeneous aquifer" has been changed to "and an isotropic, homogeneous aquifer"

Comment 8: Page 9604, L 8- L12. Is it necessary to repeat this? I think it could be skipped.

Authors' response: The reviewer has made an important observation. Accordingly, Lines 8 through 12 on page 9604 (discussion paper) have been modified to: "*WT data and Q data are collected from observation wells (Figure 5B) and stream gaging points (Figure 2), respectively*."

Comment 9: Page 9605, L 25-L 29. Why are not more assimilation times used?

Authors' response: The reviewer has raised an important point. Additional assimilation times were used, but no additional improvement was observed when 4 assimilation times were used. This is now included in the text: "*Notice that the increase of AE is lessened when observation data from multiple times are assimilated, with the best results occurring when 4 assimilation times are used. The use of additional assimilation times yielded no improvement.*"

Comment 10: Page 9609, L 20- L 22. How can the final values be so low? Could the authors further comment this? Is it related to the set-up of the verification experiments?

Authors' response: The reviewer has made an important observation. An error was found in the calculation of the sum of squared differences, and now has been corrected. The values for the updated ensembles of the first and second iteration were corrected. The text now reads: "*Quantitatively, the sum of squared differences between the model results and true system values is 95.32, 4.29, and 0.59, respectively for time = 273 days, and 99.16, 4.98, and 1.83, respectively for time = 365 days.*"

Comment 11: Page 9610, L 12- L15. Rewrite and split sentence.

Authors' response: The sentence has been changed to read: "*Assimilating Q data only slightly improved the K ensemble in relation to the true K field. Jointly assimilating Q and WT data only improved the estimate of K when data from a small number (2,4) of observation wells were assimilated.*"

Comment 12 – Table 1: The small number of layers does not seem to be suited to model unsaturated flow.

Authors' response: The number of layers stated in Table 1 does not reflect the thicknesses of each layer. These are not fully reported, but are summarized in Section 3.1: "*The subsurface is discretized by* $n_L = 10$ *layers of varying thickness, with thicknesses ranging from 0.375 m near the ground surface to 3.0 m near the aquifer base.*" Thinner layers are used near the ground surface, with thick layers (3 m) used near the base of the aquifer where unsaturated flow does not develop.

Comment 13 – Figure 2: What is the motivation to use everywhere no flow boundary conditions? Is this realistic?

Authors' response: The motivation to use no-flow boundary conditions everywhere is to follow the procedure used by Camporese et al. (2009). This is stated in Section 1.4: "*To accomplish this, the CATHY model is used in a tilted v-catchment setting, similar in design to the v-catchment used by Camporese et al. (2009)…*". We agree with this hypothesis since one can expect that, in alluvial systems, flow pathways are typically "transversal", that is, perpendicular to the stream main stem. On the other hand, we do not believe that relaxing these boundary conditions (for example, to have flow exit the aquifer through the southern edge of the aquifer) would significantly influence the results and conclusions of the study.

Comment 14 – Figure 4. The effect of cultivated vs non-cultivated fields is difficult to detect because of the random structure of the fields. Why does a line appear from Northwest to Southeast on the right map (B)?

Authors' response: It is unclear why a line of low net infiltration appears from the northwest corner to the southeast corner in the model domain. This was noticed during the modeling phase of the project, and investigation into the code that generated these values revealed no susceptibility in generating low values along this line segment. In any case, it does not influence the resulting water table elevation, and hence the results of the study.

Comment 15 – Figure 8. This is unclear to me. Why is the variance so large (unrealistically large)? Do you mean simulated WT values? Or is it correct that these are perturbed observed WT values? But why is the variance so large then?

Authors' response: The values presented in Figure 8 are perturbed observed WT values. The variance of these values is so large due to the method of calculating the perturbations:

$$E = RANDOM * CV * D$$

where D is the unperturbed water table elevation value, RANDOM is a random number from a standard normal distribution N(0,1), CV is the specified coefficient of variation, and E is the perturbation.

Comment 16 – Figure 12. Too many lines, unclear in black-white.

Authors' response: Figure 12 was designed to be displayed in color, so that the reference and update values for both the low K and high K scenarios could be presented on the same figure. As the presentation is clear in color, we have elected to keep Figure 12 unchanged.

Comment 17 – Figure 15. The AE for Fig. D is larger than for Fig. C. Does AE increase further for more iterations?

Authors' response: Yes, AE increases slightly from iteration 3 to iteration 4, although the overall spatial structure of the K field approaches the true K spatially distribution. The increase in AE is now mentioned in the text: "*The ensemble mean of the updated* Y_K *ensemble for iterations 1 through 4 is shown in Figures 15A-15D, with the AE value generally decreasing from the forecast value of 1.106 (0.755, 0.565, 0.507, and 0.518, respectively), although a slight increase occurs between iterations 3 and 4. The structure of the* Y_K *spatial distribution, however, progressively approaches the pattern of the true* Y_K *field shown in Figure 15 with each successive iteration.*"

Comment 18 – Figure 15, caption. What are the starting values?

Authors' response: The forecast value of AE is 1.106. This is now reflected in the text (see response to previous comment) as well as in the figure caption.

Comment 19 – Figure 16. Too many lines, unclear in black-white. "updated" instead of "update".

Authors' response: See response to Comment 16 above.

We are grateful to Reviewer #1 for the helpful comments and suggestions.

Comments from Reviewer #2 (Dr. Gaisheng Liu)

General Comments: The paper presents the numerical application of an inverse parameter estimation scheme (called the Ensemble Smoother) to a hypothetical surface/groundwater example. The ES is not a new idea; it was first developed by van Leeuwen and Evensen (1996). In this paper, the influence of different factors such as the number of observations, the type of data (water table or stream flow), data errors, and the uncertainty of prior information about geostatistical K model, is investigated. Particularly, the original ES is modified into an iterative procedure in order to estimate the mean and variance of geostatistical K model. The numerical results indicate that the ES scheme can provide a reasonable estimation of the K field when there is sufficient water level data. Overall, the reviewer believes that the paper makes a nice contribution to the hydrologic modeling community by presenting a detailed numerical study of ES and demonstrating its efficacy in the example problem.

The main comment is about the computational limitation of ES, as compared to other Kalman filter techniques such as EnKF. As pointed out by the authors, ES assimilates all previous model state and observation data up to the final data sampling time. This means the sizes of all the matrices involved in the calculation are increased by a factor of the number of measurement times, which will make the ES computationally difficult to apply if the real-world problem is large (millions of nodes are common in modeling practice). The authors should thus offer some remarks on the computational aspect of ES.

Authors' response: The computational time of running the ES update routine, as compared to running the CATHY simulations, are reported in the text.

For CATHY, it is reported at the end of Section 3.1: "*CPU (Central Processing Unit) time to run a single realization on an Intel® Core™2 Duo CPU @ 3.00GHz desktop computer range from approximately 20 minutes to 180 minutes, depending on the spatial distribution of Y_K.*" For the ES update reoutine, CPU time is reported at the beginning of Section 3.2: "*For these scenarios, the CPU run-time of the ES update routine is approximately 30 seconds.*"

These ES CPU times seem very affordable. The Keppenne (2000) algorithm employed in this study was designed to provide an efficient numerical strategy for updating the system state. The statement containing this information has been modified to include more information regarding the algorithm (end of Section 2.3): "*The Keppenne (2000) algorithm, which provides an efficient numerical strategy for updating the system state for the EnKF scheme and designed for high-resolution real-world climate numerical models, was modified to include model states and observation data from each assimilation time (Bailey and Baù, 2010) and used to compute Equation (4) within the ES framework. The techniques employed by Keppenne (2000) and hence inherent in the update algorithm used in this study do not require the direct assemblage of* $\boldsymbol{C}^f$*, hence saving on computer memory and preventing numerical issues.*"

Comment 1 – page 9598 – lines 1 to 3. Clarify the connection between matrices E and D.

Authors' response: The matrix E holds the perturbations that are assigned to the measurement values. The matrix D holds the perturbed values (values in the matrix E added to the measurement value). The second paragraph in Section 2.2 has been rewritten to clarify the connection between matrices E and D:

"*This correction procedure is carried out through the following Kalman Filter update equation, with the forecasted ensemble* $\boldsymbol{X}^f_t$ *corrected, or updated, at a time t using m observed data stored in a vector* $\boldsymbol{M}_t$ [*m*]:

$$\boldsymbol{X}_t^u = \boldsymbol{X}_t^f + \boldsymbol{K}_t\left(\boldsymbol{D}_t - \boldsymbol{H}\boldsymbol{X}_t^f\right) \qquad (4)$$

where $\boldsymbol{X}^u_t$ *[d x* n_{MC}*] is the updated ensemble with u denoting update;* $\mathbf{D}_t$ *[m x* n_{MC}*] holds the ensemble of perturbed values of the measurement data, with the ensemble of values for each measurement value calculated by adding a Guassian perturbation (stored in the matrix* $\mathbf{E}$ *[m x* n_{MC}*]) to each of the m observations stored in* $\boldsymbol{M}_t$*;* $\boldsymbol{H}$ *[m x d] contains binary constants (0 or 1) resulting in the matrix product* $\boldsymbol{HX}^f_t$ *that holds model results at measurement locations, and* $\boldsymbol{\kappa}_t$ *[d x m] is the so-called "Kalman Gain" matrix. In this study, observation data are sampled from a known reference state to enable assessment of the ES scheme."*

Comment 2 – page 9599 – lines 13 to 14. Clarify "off-line". Isn't it the case that in all other Kalman filter techniques, the forecast and update are sequential and thereby separable?

Authors' response: This is true, although it is possible to imbed the EnKF scheme into the numerical model so that updates can happen sequentially throughout the running of the simulation without stopping code (on-line mode). However, since this does not have to be the case, we have removed this sentence from the text.

Comment 3 – page 9603, line 14. Change "depth" to "rate". Also, it does not appear the precipitation is used as an input to CATHY. Rather, the net infiltration rate is used as input. If this is the case, please change the precipitation graph into infiltration rate graph. The precipitation graph makes people think that precipitation is a model input – then you need to consider evapotranspiration etc. in order to estimate the net infiltration rate.

Authors' response: The value shown on the graph in Figure 2 is actually a depth corresponding to the depth of net infiltration applied for the entire month. We have elected to keep "depth" in the text rather than "rate".

With regard to the infiltration rate, a similar observation was made by reviewer #1. Net infiltration is indeed used as input to CATHY rather than precipitation. This has been clarified in a number of locations in the paper:

- Section 3.1, paragraph 3: "*Forcing terms* q_{ss} *consist of uniformly-distributed net infiltration from precipitation during the months of January through March and November through December, and spatially-varying rates of net infiltration from applied water (e.g., irrigation water) in addition to net infiltration from precipitation during the months of April through October.*"
- Section 3.1, paragraph 3: "*As an example, the rates of net infiltration from combined precipitation and applied water for the month of July for one realization are shown in Figure 4B, with values ranging from 0.000355 m* day^{-1} *to 0.006 m* day^{-1} *(represented by white and black, respectively). The depth of monthly net infiltration is presented in Figure 2.*"
- Section 3.1, paragraph 4: "*The streamflow rate at the outlet cell of the catchment is shown in Figure 5B, indicating the increased discharge during the months of April through October due to increased rates of net infiltration from precipitation as well as applied water.*"
- Figure 2 has also been modified to include the axis title "*Net Infiltr. from Precip.*" rather than "Precipitation" on the inset graph.

Comment 5 – page 9608, line 9. The iterative approach is applied here only to estimate the geostatistical K model parameters. The reviewer thinks it might be worthwhile to apply the iterative approach for all the scenarios in section 3.2. Further improvement of K estimate might be possible by using the iterative approach there – instead of regenerating a new set of K realizations, the updated K fields from previous iterations can be used as initial K realizations for iterative updating.
<u>Authors' response:</u> the Scenarios we considered in Section 3.2 stem from the assumption that the geostatistical K model parameters are known. This was an intended part of the study to show results from initial attempts to improve the K estimate using water table elevation data from a catchment model. We feel that the improvement in the K fields by assimilating one set of observation data is adequate for the scope and purpose of the study. Also, improvement in the K estimate will likely be minimal since the same observation data is being assimilated. The iterative procedure will be used in future studies to demonstrate more applications. We therefore cordially decline to use the iterative procedure for all of the scenarios in Section 3.2.

Comment 6 – page 9620, Figure 2 – precipitation graph. The precipitation rates are impractically large. The number of elements shown on the figure is not consistent with table 1.
<u>Authors' response:</u> The precipitation rates used in our work are actually net infiltration rates (as specified in Comment 4 above). In addition, these are explained as depths of infiltration over the entire month, and, as such, are quite realistic rather than impractically large. The number of elements in Figure 2 reflects the surface mesh and not the entire 3D mesh. We have modified Figure 2 to clarify this. In the bottom left-hand corner, it reads: "*6724 Nodes (surface mesh)*" "*13122 Elements (surface mesh)*"

Comment 7 – page 9621 – figure 3. The font size of label too small to read. Similar suggestion for figures 5, 6 and 15.
<u>Authors' response:</u> As suggested by the reviewer, the label font size has been adequately enlarged for the Figures 3, 5A, 5B, 6, 15A, 15B, 15C, and 15D.

Comment 8 – page 9622 – figure 4B. The resolution needs to be improved.
<u>Authors' response:</u> The display of the infiltration rates is supposed to be given on a cell-by-cell basis rather than a smoother interpolated contour plot. Therefore, we have elected to not change the resolution, but rather keep the cell-by-cell values.

We thank Dr. Liu for the helpful comments and suggestions.