Reply to Referee #1:

General comments

Reply: We thank the reviewer for the constructive comments and suggestions. We revised the manuscript and thus refer to the revised manuscript.

1. "structural errors" are mentioned many times in the manuscript. However, an explicit definition is absent. What are included in the structure errors? Are they only related to the geometric error in the underlying interface between the two layers?

Reply: We understand "structural errors" as non-Gaussian deviations between the model and the measurement data, typically due to simplifications in the representation of the physical processes (more information is given, e.g., in Jaumann and Roth, 2018).

As listed in the original manuscript (P9 Line 20 – P10 Line 3), the structural errors present in this study mainly include two sources. One is the conceptual error originating from the simplification of 3D flow to 2D, the other one is mainly related to errors in the GPR observations (reflector depth and water storage). These errors are due to the varying accuracy of multi-channel GPR evaluation with different ratios of antenna separation to reflector depth, small-scale soil heterogeneity, and the interpolation of unevenly spaced data.

2. Page 6 Line 4. The Latin-hypercube was used to generate the initial ensemble. Please provide and justify the initial (prior) statistics for the hydraulic parameters. Also, do you consider the correlation between soil hydraulic parameters? This might have impacts on your inversion results, e.g., Scharnagl 2011 and Man 2016.

Reply: We are aware of the literature covering the effect of the prior statistics on the estimation of hydraulic parameters. In order not to bias the results with possibly wrong prior assumptions on the hydraulic parameters of the soils, we drew an ensemble of uniformly distributed parameters using the Latin-hypercube algorithm. Thus, the estimated parameters are solely based on the given model and the measurement data.

References: B Scharnagl, JA Vrugt, H Vereecken, M Herbst. Inverse modelling of in situ soil water dynamics: Investigating the effect of different prior distributions of the soil hydraulic parameters. Hydrology and Earth System Sciences, (2011). 15 (10), 3043-3059.

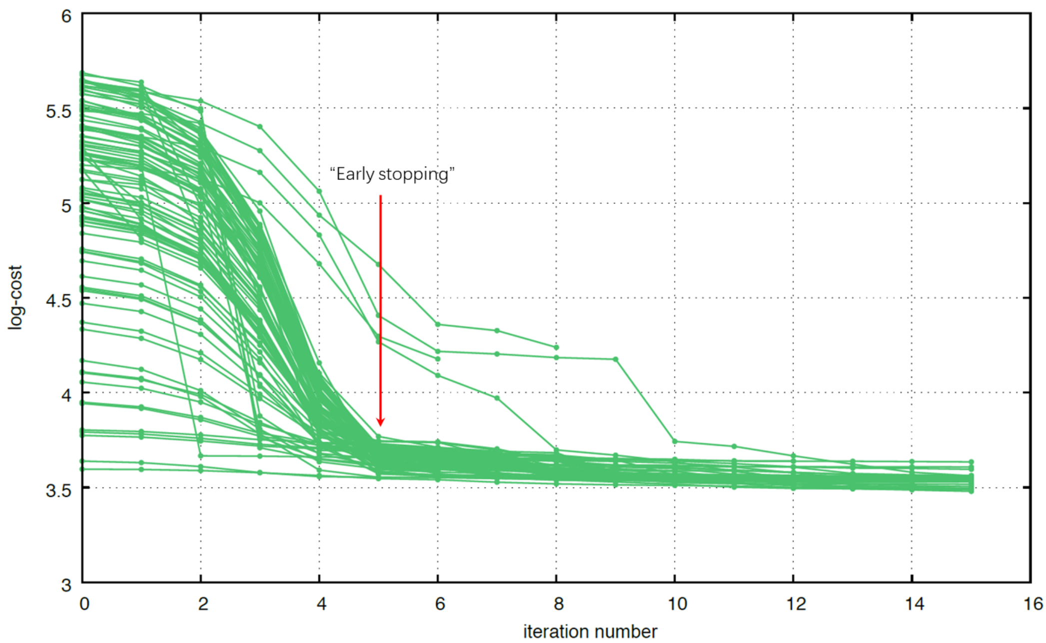
J Man, W Li, L Zeng, L Wu. Data assimilation for unsaturated flow models with restart adaptive probabilistic collocation based Kalman filter. Advances in water resources (2016) 92, 258-270

3. Please provide some information regarding the computational cost in the inversion since "efficient estimation" is highlighted in the title. For example, how many CPU hours were needed in 40 iterations in your field case. What about the computational cost in a single model evaluation if a 3D model is considered to cope with the lateral flow?

Reply: For our field case, the total time to complete the inversions of all 30 ensemble members was about 4x8x20=640 core hours (2 threads per core). The evaluation of the GPR data is comparably efficient, since the undulating surface may require a full Maxwell solver for the simulation of the GPR data increasing the computational cost by at least one order of magnitude.

A 3D model could deal with the lateral flow, however the corresponding computational cost multiplies approximately by the number of grid cells in the third dimension. Thus, we decided to proof of our approach using a 2D model. Certainly, going 3D requires scaling the computational power, however it does not require additional concepts to what is presented in this study.

4. Page 6. The early stopping may cause the overestimation of uncertainties. How do you choose an appropriate iteration number in practical applications? Please clarify.
Reply: Commonly, the "optimal stopping" criterion (stop when meeting one of the the convergence criterions) should be enough for ideal conditions, but overfitting might happen when modelling uncertainties are notable. To avoid overfitting, we used a two-step criterion for the field study. The complete procedure is that the "optimal stopping" criterion is applied with a number of iterations up to 40 at first, then the "early stopping" iteration number is identified after an analysis of the convergence behavior of the parameter distribution. As a rule of thumb, for the "early stopping", we analysed the parameters of the according iteration number (e.g., 5) where the spreading of the cost values becomes stable as shown in the following figure. Generally, the "optimal stopping" criterion should be applied once the structural errors are alleviated in the field study.



We clarify this in the P10 lines 4-10 as "Hence, a two-step procedure is applied in this study. Initially, we used the "optimal stopping" criterion only considering measurement precision and it resulted in a large number of iterations as well as overfitting. After an analysis of the convergence behaviour of the parameter distribution, we identified that overfitting could be avoided by using the "early stopping" criterion and evaluating the output of the 5th iteration. Note that the "optimal stopping" criterion should be applied once the structural errors are alleviated in the field study."

5. Please shorten the caption of figure 4 since it is rather long.
Reply: It is rephrased as following.
"Figure 4. Effective hydraulic properties estimated with the proposed approach for the field study (upper panel) and the synthetic study (lower panel). The grey curves in all subplots

represent the estimated hydraulic functions from ensemble members using the “early stopping” criterion. The black curves in (a) and (b) are derived from the median parameters of the best 68 members, while the black curves in (c) and (d) are the same members but using the “optimal stopping” criterion. The red curves in (c) and (d) are derived from the true parameter given in Table 2. The histograms in (a) and (c) (blue histogram, the same in Fig. 6 and Fig. 7) mark the covering range of the mean water content evaluated from the GPR observations.”

6. Figure 5 shows significant unresolved biased errors. If I understand correctly, is it possible to alleviate this problem by incorporating geometric stratal errors in the architectures? To be more specific, it seems that all the inversions are based on the same interface (shown in Figure 2). Can you use an interface ensemble instead? This is similar to the treatment of using initial parameter ensemble in your inversion.

Reply: The remaining deviations between the model and the measurement data are related to the structural errors which are not restricted to the geometric stratal errors, but also include errors concerning water storage estimation, analysis of the GPR data, and the conversion from 3D to 2D. This can be analysed with a Bayesian total error analysis (BATEA; Kavetski et al., 2002, 2006) by creating ensembles of different models that can represent these structural errors and using this ensemble for parameter estimation. However, this is a major effort that goes well beyond the scope of this study.

Kavetski, D., S. Franks, and G. Kuczera (2002), Confronting input uncertainty in environmental modelling in calibration of watershed models, in Water Sci. Appl. Ser., vol. 6, edited by Q. Y. Duan, et al., pp. 49–68, AGU, Washington, D. C.

Kavetski, D., G. Kuczera, and S. W. Franks (2006), Bayesian analysis of input uncertainty in hydrological modeling: 1. Theory, Water Resour. Res., 42, W03407, doi:10.1029/2005WR004368.