

Interactive comment on “Bayesian inverse modelling of in situ soil water dynamics: using prior information about the soil hydraulic properties” by B. Scharnagl et al.

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Received and published: 21 July 2011

Reply to general comments

We highly appreciate the many insightful comments provided by the four referees. These comments were very helpful in sharpening the focus of the present study and in improving the traceability of the methods used.

It was clearly not our intention to convey a wrong impression about the novelty of this research, and we apologize if the reader of the discussion paper may have left with

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this impression. In this context, we are especially grateful for pointing our attention to the Hou and Rubin (2005) paper, which is highly relevant to the work presented in the discussion paper, but unfortunately, of which we have been unaware before.

We do not agree, however, that the discussion paper does not present any new findings, and that the use of prior information has been extensively used before, as suggested by some of the referees. We agree that there is a lot of general information in the statistical literature on the impact of various prior distributions. We also agree that the use of prior information is quite frequent in the field of groundwater hydrology and hydrogeophysics. However, there are only very few soil hydrological publications that have studied the role of an informative prior distribution of the soil hydraulic parameters in estimating the soil hydraulic properties from water content data. This approach, even though appealing from a conceptual point of view, has not become common practice in soil hydrology, as demonstrated by the review of literature provided in the "Introduction" of the discussion paper. In fact, very little is known about the effect of various prior distributions on the posterior estimate of the soil hydraulic parameters. Our study aims at filling this gap. In particular, we present an approach to derive the correlation structure of the soil hydraulic parameters predicted by the ROSETTA pedotransfer function. The results of our study suggest that information on parameter correlation is highly beneficial because it substantially improves the identifiability of the soil hydraulic parameters.

We added a paragraph to the "Introduction" of the revised manuscript where we refer to related work in groundwater hydrology and hydrogeophysics (e.g., Carrera and Neuman, 1986, *Water Resour. Res.*, 22:199-210; Woodbury and Ulrych, 1993, *Water Resour. Res.*, 29:2847-2860). In addition, we will present and discuss related work in the field of soil hydrology that makes explicit use of prior information about the soil hydraulic parameters (Wang et al., *Vadose Zone J.*, 2:297-312, 2003; Mertens et al., *J. Hydrol.*, 294:251-269, 2004; Hou and Rubin, *Water Resour. Res.*, 41:W12425, 2005). In the revised manuscript, we put our work in context of these studies and

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pointed out more clearly the novelty and main findings of our approach. In addition to these changes, and as suggested by two referees, we modified the title of the revised manuscript in order to better reflect the actual content of the paper. The new title is “Inverse modelling of in situ soil water dynamics: investigating the effect of different prior distributions of the soil hydraulic parameters”. We also revised the abstract to better reflect the actual focus and content of the present study.

Reply to comments of anonymous referee #1

1.1) ... However, the authors have overstated the novelty of using the prior and investigating the impact of prior, since they have been explored, for example, by Hou and Rubin (2005) ...

See reply to general comments.

1.2) First, the definition of "prior" in this paper is confusing. ...

We agree on that the term "prior information" needs clarification. In the discussion paper, we considered the information about the soil hydraulic properties derived from information about soil texture (percentages of sand, silt, and clay) using the ROSETTA pedotransfer function as "prior information". It is "prior" in a sense that the information about soil texture is much more readily available than detailed information on soil water dynamics, from which the soil hydraulic properties can be inferred. In addition, information on soil texture is typically available before a time series of soil water state observations is obtained. Also, the information on soil texture does not necessarily have to stem from direct measurements, as it was the case in our study. Information on the soil textural class of a given site can often be derived from available soil maps. We added this explanation to the revised manuscript.

1.3) Second, the authors argue that the in-situ soil water content data alone does not

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give reliable estimates so that they need informative prior. At the same time, they say that different (biased) prior did not have any effect on the results so that their method is robust. ...

We do not think that these two sentences are contradictory, as suggested by the referee. However, the two findings summarized in these sentences may indeed need further explanation and discussion to avoid any potential misconception. The misconception probably arises from what one might understand under “biased” prior. In the present study, the magnitude of the bias was chosen based on the uncertainty in the ROSETTA prediction (with the “true” parameter combination used to generate the data falling outside the 95 % confidence interval of the ROSETTA prediction). This is, in our view, a realistic but still moderate form of bias. As shown in the discussion paper, under these conditions our approach of using prior information is robust. Clearly, another situation occurs if the magnitude of the bias is so large that the prior distribution actually becomes incompatible with the information contained in the observational data, as illustrated and discussed in Hou and Rubin (2005). In this situation, any approach of using prior information is very likely to fail. In practice, however, this failure will become evident from inspection of the posterior distribution, as shown in Hou and Rubin (2005). We added a paragraph in the “Results and discussion” section of the revised manuscript, in which we discussed and clarified this issue.

1.4) The way to determine the correlation among parameters in the prior distribution was questionable. ... It does not account the correlation created by the pedotransfer function (PTF) through ROSETTA. ...

In fact, the opposite is true. Our approach to derive the covariance matrix of the ROSETTA predicted parameters explicitly accounts for the correlation created by the PTF. It does not account for the actual variability in the measured percentages of sand, silt, and clay. Moreover, we think that our approach of generating a random sample of soil texture data is adequate because it naturally accounts for the correlation between the percentages of sand, silt, and clay. Because of measurement errors, these mea-

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surements typically do not add up exactly to 100%. The ROSETTA program accounts for this fact by allowing for an error tolerance of 1% on the sum of sand, silt, and clay percentages given as input variables. We revised the description of our approach to derive the covariance matrix accordingly and provided some additional explanation that helps to follow this method.

1.5) It would be better to say "investigating the impact of prior" rather than "using prior".

We changed the title of the revised manuscript accordingly. The new title is "Inverse modelling of in situ soil water dynamics: investigating the effect of different prior distributions of the soil hydraulic parameters"

1.6) Many definitions and phrases are informal and vague ...

We revised the discussion paper and replaced those phrases.

1.7) Symbols (e.g., L, Ks) are used before defining them.

We resolved this issue in the revised form of the manuscript.

1.8) What is the uncertainty range of these measurements and variability within the model domain?

Soil texture within the experimental plot was fairly homogeneous. Measured percentages of sand, silt, and clay had a standard deviation of 1% each in the top layer and 2% each in the bottom layer of the profile. The magnitude of the standard deviation is identical or very close to the standard error of the method used for texture analysis (wet sieving followed by the pipette method). Given this information, it is reasonable to assume that each of the two layers is homogenous in terms of its soil hydraulic properties. We included this information in the revised manuscript.

1.9) It is necessary to have a physical reason to justify homogeneity rather than just for convenience.

The assumption of a homogeneous soil profile was based on available information

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about the vertical distribution of soil texture, as given in the discussion paper. According to these data, there is only a slight difference in soil texture between the top and the bottom layer of the profile. A preliminary analysis using ROSETTA to predict the soil hydraulic parameters for both the top and the bottom layer showed that both layers are expected to be almost identical in terms of their soil hydraulic properties. Based on this preliminary analysis, we assumed that this minor difference in soil hydraulic properties can be neglected and that the profile can be assumed to be homogeneous. This information was included in the revised manuscript.

1.10) *Although it is clearly defined, using \hat{x} for measured observations still seems inappropriate, because hat is always used for estimates in statistics.*

We changed the notation accordingly.

1.11) *"To formulate ... the model residuals" is not a precise statement but very vague.*

...

We rephrased this sentence accordingly.

1.12) *It is important to state what ε physically means (measurement errors ?) and why one can justify that they are independent and identically distributed.*

Model residuals result from observational and modelling errors. The assumption of independent, identically, and normally distributed model residuals should be considered a working hypothesis. This hypothesis has proven useful in many inverse modelling applications, including soil hydrology. Its validity, however, should be tested a posteriori. Unfortunately, this is not current practice in the soil hydrological literature. In the present study, this testing was done using diagnostic plots (Fig. 9). If any of these plots would have indicated that these assumptions do not hold, the working hypothesis would have to be rejected and the likelihood function would have to be revised. See also reply to comment 4.5.

1.13) *Equation (8): \hat{y} should be replaced by \hat{y}_i .*

We changed Eq. (8) of the revised manuscript accordingly.

1.14) Equation (7) is a simple subtraction of vectors such that $\varepsilon_i = \hat{y}_i - y_i(\vec{x}_1, \vec{x}_2)$.

We changed Eq. (7) of the revised manuscript accordingly.

1.15) $\vec{\varepsilon}$ should be a function of \vec{x}_1 and \vec{x}_2 , $\vec{\varepsilon}(\vec{x}_1, \vec{x}_2)$.

We changed Eq. (7) of the revised manuscript accordingly.

1.17) The likelihood formation is wrong.

The likelihood function defined in Eq. (8) is correct. It results from integrating out the standard deviation of the residuals, σ_ε^2 , after assuming a Jeffreys (noninformative) prior distribution for σ_ε (e.g., Box and Tiao, 1992, Kavetski et al., Water Resour. Res., 42:W03407, 2006). We provided this additional information in the revised manuscript to facilitate the traceability of the Bayesian approach used in this study.

1.17) Equation (9): The equation assumes independence between \vec{x}_1 and \vec{x}_2 in prior. It needs to be justified.

The assumption of independence between \vec{x}_1 and \vec{x}_2 as stated in Eq. (9) is a simplifying assumption. Based on the underlying physics of the system, we may expect that \vec{x}_1 and \vec{x}_2 are correlated. This expectation is corroborated by the correlation between these various parameters found in the posterior sample (e.g., Fig. 4). In practice, however, it is not possible to translate the prior information about the soil hydraulic parameters \vec{x}_2 into an informative prior of pressure head at the lower boundary \vec{x}_1 . In this situation, assuming independence between \vec{x}_1 and \vec{x}_2 seems to be justified. We added these considerations in the revised form of the manuscript.

1.18) "This posterior distribution summarizes what we know about the parameters" is informal.

We revised this sentence.

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1.19) *"we can do better than this" is very informal. ...*

We revised this sentence, as well. In addition, we made reference to the Hou and Rubin (2005) paper here.

1.20) *The authors need to justify why they chose -250 and -50cm for the bounds.*

The choice of the bounds was based on the available information about the depth of the ground water table, as given in the text, and the assumption of an approximate hydrostatic equilibrium between the lower boundary of the simulation domain and the ground water table. We included this justification in the revised manuscript.

1.21) *We cannot omit the uniform prior from the posterior distribution, because the prior still affects the posterior such that the posterior probability density outside of the bounds is zero.*

We are grateful for pointing our attention to this inconsistency in the description of the MCMC method. The reason for this is that the implementation of the DREAM_(ZS) algorithm does not allow for sampling outside of some predefined parameter bounds. Using this implementation, a uniform prior does not need to be evaluated and can therefore be omitted from Eq. (9). However, we agree that this account is formally inconsistent. We revised the corresponding parts of the discussion paper accordingly and removed these inconsistencies. However, we like to point out that the use of predefined parameter bounds is not a limitation of DREAM_(ZS). It is rather based on efficiency considerations.

1.22) *Uniform distributions also require explicit prior knowledge for the upper and lower bounds.*

We also agree on this point and apologize for the incorrect statement. We modified this sentence accordingly.

1.23) *There are many other MCMC schemes (e.g., Gibbs sampling) which are widely used.*

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We rephrased this sentence accordingly.

1.24) The next position of the chain should also depend on the data, in addition to the current position, as is shown in Equation (11).

We modified Eq. (11) accordingly.

1.25) ... Again, the authors need to justify use of a particular distribution based on physical processes or observations; otherwise the inverted results are meaningless.

We agree that the expression “A normal distribution is computationally easy to implement...” is misleading and will therefore be removed. The justification for the use of the multivariate normal distribution as a prior model was provided by quantile-quantile plots and pairwise scatter plots of the VGM parameters predicted from the random sample of soil texture data (Step 2 of the proposed algorithm). For reasons of conciseness, however, we did not show these two diagnostic plots. These diagnostic plots clearly illustrate that the two preconditions that justify a multivariate normal distribution were met: (i) marginal normal distribution of each VGM parameter, and (ii) linear correlation between the various VGM parameters. We clarified this point in the revised manuscript, providing some additional explanation.

1.26) The authors need to state why they chose multivariate normal prior distribution.

See reply to comment 1.25.

1.27) "0.25 % was shown to work well in practice" needs a reference. In addition, the authors need to state what $\vec{\sigma}_f$ means physically (e.g., measurement errors and/or variability).

This expression is indeed misleading and was modified. Actually, we chose a value of 0.25 % based on a preliminary analysis. $\vec{\sigma}_f$ is used to draw a random sample of sand, silt and clay percentages, which in turn is used to predict the VGM parameters (Step 1 in the proposed algorithm). This step is conceptually similar to approximating the sensitivity (Jacobi) matrix used to evaluate parameter uncertainty and correlation

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in the classical first-order approach (e.g., Mishra et al., 1989, J. Hydrol. 108:1-18). The so-obtained random sample of VGM parameters drawn in the immediate vicinity of the mean parameter values $\vec{\mu}_{\vec{x}_2}$ (Step 2 of the proposed algorithm) can then be used to estimate the correlation structure of $\vec{\mu}_{\vec{x}_2}$ (Step 3 of the proposed algorithm). Compared to the classical first-order approach, the Monte Carlo approach we used has the general advantage that the underlying assumptions can easily be tested using diagnostic plots (see also reply to comment 1.25). We added these explanations to the revised manuscript to facilitate understanding of the proposed algorithm.

Reply to comments of anonymous referee #2

2.1) However, from the conceptual and theoretical point of view, the paper does not bring any new insights.

We do not agree on that the discussion paper does not provide any new insights. A new aspect of the present study is the incorporation of parameter correlation in the formulation of the prior distribution. To this end, we presented an approach to derive the correlation structure of the ROSETTA predicted parameters, and we demonstrated that this information is particularly valuable because it substantially improves parameter identifiability. To our knowledge, this issue has not been treated in the literature before. See also reply to general comments.

2.2) Many of the issues raised by the paper (e.g., use of Bayesian theory and relevance of priors in predictions) has been tackled in the past.

See reply to general comments.

2.3) However, no substantial conclusions with conceptual substance were reached.

See reply to general comments.

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2.4) *The authors explain the discrepancy between laboratory and field scales however, the authors did not mention anything related to scales of heterogeneity. ...*

We modified this paragraph as suggested by the referee.

2.5) *... A lot of these issues mentioned in this paragraph are not novel and have been tackled in the past. ... Reading this paragraph cited in this comment gives the "impression" that the topic is being treated for the first time.*

See reply to general comments.

2.6) *... The above sentence gives the impression of novelty and I believe the authors should consider re-phrasing it.*

We rephrased this sentence accordingly.

2.7) *The authors justify the choice for the multivariate uniform distribution model (what they denote as prior 1) however justifications are still needed for prior 2 and 3.*

We included this justification in the revised manuscript. See also replies to comments 1.25 and 1.27.

2.8) *... Please add some references to support this statement.*

We added some references here, as suggested by the referee.

2.9) *Although out of the scope of the paper, I think the authors should consider adding a sentence or two (perhaps expanding the discussion) related to the use of prior information to address issues related to model uncertainty. ...*

As illustrated in the present study, the use of informative prior distributions improves the indenifiability of the soil hydraulic parameters from observational data that contain insufficient information to warrant accurate and precise parameter estimation. In general, we may expect that the use of an informative prior distribution increases the sampling efficiency in stochastic inverse modelling (e.g., Flores et al., 2010, Water Resour. Res.,

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46:W04506), which leads to a reduction in the computational cost. The same approach can easily be applied in Bayesian model averaging, such as that proposed in Neuman (2003, Stoch. Env. Res. Risk A., 17: 291-305). In general, we may expect that the improvement in parameter identifiability may affect the outcome of the Bayesian model averaging. The magnitude of this effect, however, is difficult to predict. We agree with the referee on that these kinds of model uncertainty issues are a fascinating topic. However, we feel that it is too far out of the scope of the discussion paper and should be addressed in depth in a separate study.

2.10) Please provide the year of the reference “Ritter et al.” in the text.

We provided the year of the reference in the revised manuscript.

2.11) The sentence “In addition, we can infer predictive uncertainty by propagating each realization of the posterior distribution ...” is a bit confusing. ...

This expression is indeed incorrect. It should read "...propagating each realization of the posterior sample...". We modified the revised manuscript accordingly.

2.12) What does it mean “create the prior pdfs”? ...

This expression is imprecise and confusing. It should read “infer the prior pdfs”, as suggested by the referee. We made these changes to the revised manuscript.

Reply to comments of anonymous referee #3

3.1) As a general comment I should say that this paper deals with issues that were dealt extensively in previous works, but without providing proper references. ...

See reply to general comments.

3.2) ... Going over these items one by one, I do not get the sense that these goals are

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worthy of pursuing because (1) they were answered in a broad context of statistics and the answers are well known; (2) I do not think that there is a question about "how much prior" makes sense as presented. ...

We do not think that the answers to these questions are well known. Only very few studies have used prior information on soil hydraulic parameters in a formal Bayesian way. Moreover, none of these studies has incorporated information about parameter correlation in the formulation of the prior and investigated its effect in a systematic way. We agree with the referee on that the questions that summarize the scope of our study need to be reformulated, especially the one about "how much prior information is needed", as mentioned by the referee. We revised this part of the discussion paper to better reflect the actual focus and content of the manuscript.

3.3) The following statement is problematic: "... It is misleading and unfair because of the enormous body of work existing in this area that is ignored here.

See reply to general comments.

3.4) Next, how does one define "sufficient" and what is meant by "reliable estimates"?

...

We agree on that our use of "reliable estimation" is imprecise and indeed misleading. We also agree on the definition given by the referee: The reliability of an estimate is associated with accurate quantification of its uncertainty. Instead of "reliable estimation" we will use the term "accurate and precise estimation", which we define as an estimate associated with a 95 % confidence interval that is reasonably small and covers the true value of the estimated parameter. The information contained in the observational data is "sufficient" if it warrants the accurate and precise estimation of all parameters of interest. We revised the discussion paper accordingly and also provided these definitions in the revised manuscript.

3.5) "... That's grossly inaccurate. See my comments above and references regarding

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rational selection of priors. The body of literature in statistics on the proper choice of priors is huge.

See reply to general comments.

3.6) "... " This statement does not define what is meant by effective properties, except to suggest that they are related to the arithmetic averages of the soil moisture. ..."

We defined the term "effective properties" on p. 2021, l. 26-28 of the discussion paper, following the definition given in Vereecken et al. (2008). We agree with the referee that effective properties do not exist for heterogeneous systems under transient boundary conditions. We think, however, that our approach of estimating effective soil hydraulic properties is justified by the apparent homogeneity of the simulation domain, as outlined in our replies to comments 1.8 and 1.9. The apparent homogeneity in context with the definition of effective properties justifies the averaging of the spatially distributed water content observations. In fact, this approach of estimating effective soil hydraulic properties is frequently applied in soil hydrology. All studies we cited in our review of literature (p. 2022-2023) apply this same approach. It is also frequently used on even much larger spatial scales using remote sensing data to estimate the effective soil hydraulic properties (e.g., Montzka et al., 2011, J. Hydrol., 399:410-421).

3.7) The paper provides only limited information on the site. It also does not provide information that could be used to justify the assumption of one-dimensional flow.

We added more information about the experimental site in the revised manuscript, as outlined in our replies to comments 1.8, 1.9, and 4.2. The experimental plot is located at the bottom of a gently sloping agricultural field, having a maximum slope of about 3°. The experimental plot itself is plane. This geographical setting makes lateral flow very unlikely to happen and justifies the assumption of one-dimensional, vertical flow. We included this information in the revised manuscript.

3.8) Focusing on near surface measurements (6 cm depth) is problematic on several

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counts: (1) soil is quite disturbed (root and biological activity and weather) and it questionable whether the priors are at all applicable (2) effects of weather (like temp variations) are ignored, and there is no doubt that at such depths they must be recognized.

The "disturbance" mentioned by the referee caused by biological activity and drying/rewetting will in general lead to formation of aggregates, macropores and other structural features, commonly referred to as soil structure. For obvious reasons, these biological and physical processes are most pronounced near the surface. We like to point out, however, that soil structure is a most natural feature of field soils and that some degree of soil structure is typically present throughout the soil profile. In our view, there is no reason why the soil hydraulic properties predicted by ROSETTA, and hence, the prior distributions inferred from this prediction, should not be applicable to a field soil that has structural features. In fact, the results of our study suggest that the prior distributions conform very well to the information contained in the water content information.

We are aware of the effect of temperature on the apparent dielectric permittivity, and consequently, on TDR measurements of soil water content. To test whether there is a temperature effect apparent in our TDR data, we analyzed the spatially distributed measurements for a temporal trend. Because soil respiration and soil temperature (at 6 cm depth) measurements were taken simultaneously with soil water content measurement at the same locations, a complete measurement cycle took about three hours. While the soil temperature data showed a well pronounced trend over this time period, there was no significant trend in the soil water content data. From this we concluded that the temperature effect in the TDR data is negligible.

3.9) What is the justification for this assumption? In fact, it is not applicable generally. What would be the impact of this assumption on the results?

See replies to comments 1.12 and 4.5.

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Reply to comments of anonymous referee #4

4.1) The title is quite generic; also, the abstract does not add proper information to understand the key results of the paper. It is necessary to explicit, at least in the abstract, which soil data are used. ...

We included the missing information about the soil data in the abstract. We also changed the title of the revised manuscript. The new title is “Inverse modelling of in situ soil water dynamics: investigating the effect of different prior distributions of the soil hydraulic parameters”.

4.2) Some references, figures or tables with details on the field site could be useful. ...

We included a figure showing the spatial distribution of the measurement points in the revised manuscript. The pressure had at the lower boundary was not measured but estimated simultaneously with the soil hydraulic parameters, as explained in Section 2.2.4 of the discussion paper. See also replies to comments 1.8 and 1.9.

4.3) The covariance matrix of prior soil parameters is computed with an arbitrary covariance matrix of the sand, silt and clay percentages. ...

See reply to comment 1.27.

4.4) The presentation and discussions of the results is very long and could be shortened. ...

We agree on that the main finding of our study — the importance of including parameter correlation in the prior distribution — should be emphasized. We modified the “Results and discussion” section accordingly. In this context, we also revised the manuscript for content that can safely be removed without loss of comprehensibility and readability.

4.5) In fact the comments to figure 7 show that there are some outliers, which are apparent on the tails of the distribution in figure 9c. ...

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In our view, the two outliers that are evident in Fig. 7 and 9c do not invalidate the Gaussian likelihood function used in this study. In general, the quantile-quantile plot shows a good agreement with the hypothesis that the residuals are approximately normally distributed, except for the two outliers. See also reply to comment 1.12.

4.6) *Add (2011) after Steenpass et al.*

We added the year of the reference.

4.7) *Is "expertise" the proper word, or should it be replaced with "experience"?*

"experience" is the proper word here, as suggested by the referee. We modified the revised manuscript accordingly.

4.8) *I would erase lines 2 to 5 of page 2045, because it is absolutely obvious that one cannot estimate in a confident way the residual and saturation water content if dry and wet conditions are not monitored!*

The two sentences were removed from the revised manuscript.

4.9) *Erase the sentence "The grey lines...the data."*

This sentence was also removed.

4.10) *Is it possible to draw an estimated error bar for the measured water content? This should include the uncertainties related to the Topp's formula and to the spatial variability.*

We added bars to the mean values plotted in Fig. 7 showing the 2.5% and 97.5% quantiles of the spatial distributed soil water content observations. These 95% intervals convey an impression of the spatial variability of the measurements. They integrate the uncertainty resulting from the use of Topp's equation as well as other sources of measurement error.

4.11) *Some observations fall outside the 95% prior distribution bounds. Could you*

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comment on this?

The reason for this is that both prior and posterior bounds in Fig. 8 show the uncertainty in the soil hydraulic functions due to uncertainty in the soil hydraulic parameters only. They do not include observational and model errors. This is the reason why some observations fall outside the uncertainty bounds. We added this explanation to the revised manuscript.

4.12) What is "partial" autocorrelation? Which are the measurement units of lag? ...

The partial autocorrelation of the model residuals separated by a given lag is the autocorrelation of these residuals not accounted for by lags smaller than the given lag. Partial autocorrelation is typically used to identify the order of an autoregressive model of a time series. However, as we came to realize just recently, the autocorrelation (not the partial autocorrelation) would actually be the more appropriate measure in the present case. This is why we present a plot of the autocorrelation function in the revised manuscript instead of the partial autocorrelation function shown in Fig. 9a. Both functions differ only marginally, and this does not alter any of the results or conclusions. The "lag" is basically the number of measurement dates separating two model residuals, as suggested by the referee. In the present study, only 29 measurement dates were available, which is on the edge of being an acceptable number for the calculation of the autocorrelation function. This relatively small number of measurement dates is reflected in the relatively wide 95 % significance interval shown in Fig. 9a.

Interactive comment on Hydrol. Earth Syst. Sci. Discuss., 8, 2019, 2011.

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