Kalman filters for assimilating near-surface observations in the Richards equation – Part 2: A dual filter approach for simultaneous retrieval of states and parameters
H. Medina, N. Romano, and G. B. Chirico

Reply to Referee 1

We thank Referee#1 for his/her valuable review. We take Referee's comments into careful consideration while revising the manuscript. Below we provide our detailed replies.

Ref#1

This paper presents a dual Kalman filter strategy for the update of states and parameters in the Richards equation, based on the assimilation of near-surface pressure head or soil moisture. The system state, accounted for in terms of either pressure head or soil moisture, is updated by the classic Kalman filter (KF), while the Unscented Kalman filter (UKF) is used to update the soil properties (hydraulic conductivity and soil retention curves parameters). Although the topic is certainly of interest for the hydrological community, I have a number of serious concerns that in my opinion must be addressed before the paper can be published.

Overall, it seems to me that the conclusions of the study actually represent a step back in the topic of data assimilation for nonlinear systems, as the strategy is largely based on the classic Kalman filter applied to a linearized numerical scheme for the solution of the Richards equation. Therefore, the Authors are trying to challenge the nonlinearity of the problem by adapting the system to the assimilation algorithm and not vice versa, which is the common strategy. This is of course legit and the choice cannot be questioned "a priori". The problem, in my opinion, is that the results, contrary to what claimed by the Authors, are neither convincing nor encouraging. I will provide more details in the following, under the section "specific comments".

Reply

The companion paper (Chirico et al., 2012) showed that the CN numerical scheme, although less numerically efficient than NL (which is implemented in the most popular soil water dynamics simulation software), when combined with the classic Kalman Filter (SKF) provides assimilation performances similar to those obtained with a UKF-NL algorithm, with much less computational drawbacks. Certainly, this advantage is relevant as far as system dimensionality is limited, such as the soil column examined in this study. We will acknowledge in the paper that other assimilation strategies, such as the EnKF or UKF, which do not imply an explicit formulation of the covariance propagation as in the case of the SKF, are more feasible for large scale applications.

Ref#1

Another major issue of the paper is that the methods are not described comprehensively.

I refer in particular to the UKF, whose description is rather confused and difficult to follow. As far as I understand, UKF theory is not straightforward and its application to the Richards equation represents one of the major novelties of the paper: for these reasons I would expect a more precise description, including the details of the several parameters that need to be tuned in order to obtain a satisfactory performance of the assimilation framework. These parameters are hastily discussed in section 5.5, but this is not sufficient: a reader who wanted to reproduce the same results would not be able to do so only with the information provided in the paper. Again, more details follow below.

Reply

The introduction will be rewritten by giving emphasis to the novelty of the study, which is the application of the UKF for retrieving parameters in dual state-parameter assimilation algorithm.

The UKF will be fully described as well as the parameters employed for its implementation.

Ref#1

Specific comments

Page 13331, lines 6-13: given that the paper deals with a 1-D model of unsaturated flow, this discussion is not much relevant and can be shortened. This would allow adding more details on the subsequent paragraph, as reported in the following point.
Page 13331, lines 15-18: this paragraph is much more relevant than the previous and thus should be expanded with a proper number of citations of studies focused i) on retrieving states only and ii) on retrieving states and parameters.

Reply

We will change Page 13331 accordingly.

Ref#1

Page 13332, lines 17-20: this statement cannot be generalized. Other KF-based algorithms, such as the ensemble Kalman filter (EnKF), have been proved to be efficient when implemented with a nonlinear numerical solver of the Richards equation. For instance, Camporese et al. (WRR, 2009) reproduced the same experiments of Entekhabi et al. (1994) and Walker et al. (2001) with a good retrieval of the system state and without any problem of numerical stability.

Reply

We agree with Referee 1. We propose to change the statement as follows: "*Chirico et al. (2012) showed that the state retrieval in a low dimensional problem of soil moisture assimilation can be efficiently achieved by coupling a Crank-Nicolson linear numerical integration scheme of the Richards equation with a standard KF (SKF) algorithm"*.

Ref#1

Page 13333, line 13: "weights"? Perhaps do you mean "parameters"?

Reply

Yes, we intend parameters. We adopted the initiative of Wan and Nelson (2001), and Nelson (2000) who indistinctly used both terms.

Ref#1

Page 13333, eq. (1): I believe that u and v should be at the current time step k. Also, the meaning of the symbol "^" should be stated right after the equations, while it is (probably, see related technical correction) currently placed much later, at line 7 of page 13334.

Reply

Yes, it is formally more correct to assign *u* and *v* to the current time step *k* in Eq. 1. We will carefully illustrate the meaning of the symbols.

Ref#1

Page 13334, eq. (5) and elsewhere in the manuscript: you cannot use the symbols "^" and "-" together, as the former means posterior and the latter prior. Please remove "^" from all the prior variables.

Reply

Data assimilation studies use dissimilar notations. One widely extended (Maybeck, 1979; Julier and Uhlman, 1996; van der Merwe, 2004, and others), adopted by us, is to use the symbol "^" just for indicating "estimated". At the same time many authors employ "-" and "+" for indicating prior and posterior mean, respectively (Maybeck, 1979, De Lannoy et al., 2007, Reichle, et al., 2002). We used the notations adopted by Wan and Nelson (2001) and van de Merwe, (2004), indicating with the "-" (e.g., $\hat{\boldsymbol{x}}_k^-$) the a priori mean estimate and, in its defect (e.g., $\hat{\boldsymbol{x}}_k$), the a posteriori mean estimate.

Ref#1

Page 13336, eq. (16): this equation should be either demonstrated or given a proper reference.

Reply

Van Der Merwe (2004) provides an optimization perspective of the sigma point Kalman filter estimation, similarly to what Nelson (2000) and Wan and Nelson (2001) do for the dual extended Kalman filter methods. Nevertheless, we prefer to remove Lines 1-5, page 13346, including Eq. (16); it is scarcely relevant and creates confusion.

Ref#1

Page 13336, line (15): the expression S_i = {mi_i, W_i, i = 1…L} is erroneous and misleading. It should be i = 0…2L and it should be stated that the actual sigma points are the variables W_i, while mi_i are the weights used for computing mean and covariance.

From page 13337, line 7 to page 13339, line 6: all this part is obscure and rather incomprehensible and must be rewritten. Also, when writing down the equations, please remember to define every variable (e.g., missing definitions currently include L_w and Yˆz_k|k-1 in eq. (24), P_wk_yk in eq. (25), R_ek in eq. (26), etc).

Reply

It is true; the correct expression should be:

$$\mathbf{S}=\{\mu_i,\boldsymbol{\mathcal{W}}_i,\ i=0\ldots 2L\}$$

In order to avoid confusion to the reader we would instead prefer to follow the definition of Julier and Uhlmann (2004): "a set of sigma points **S** consists of 2L+1 [in our case] vectors and their associated weights".

As suggested, we will rewrite section 2.1.2.

Ref#1

Page 13344, lines 11-12: "zero gradient" boundary conditions mean no-flow and not "free drainage". Please clarify what boundary conditions were used in the simulations.

Reply

The complete sentence written at page 13344, lines 11-12 is: "*the bottom boundary condition is set by a zero gradient of the soil water pressure head, also known as free drainage*". This sentence is correct, as free drainage corresponds to the condition of unit gradient of the total potential head $H=h-z$ (z is the soil depth taken positive downward), i.e. zero gradient of the pressure head (h).

Ref#1

Page 13345, line 1: please clarify what do you mean by "heterogeneous discretisation". Does that mean that the layer thickness is not constant? If so, please give more details.

Reply

Yes, we do intend that the computational compartments are not uniform along the soil column. We will provide details in the revised manuscript.

Ref#1

Page 13345, lines 23-24: stating that a variance of 10ˆ3 cmˆ2 is ten times the initial state does not make any sense, as you are comparing square cm with cm. You should refer to the standard deviation (_32 cm) or coefficient of variation, which in this case is_1/3.

Reply
We will correct our statement, thank you. The coefficient of variation is 10.5% with respect to the initial state (-300 cm).

Ref#1
Page 13345, line 28: "is updated as a diagonal matrix", please rephrase this sentence.
Reply
We will change the sentence as follows: *"The observation noise covariance matrix is set equal to 2% for the diagonal elements and zero for the off-diagonal elements".*

Ref#1
Page 13346, eq. (43): I believe that using the Mean Absolute Error would be more desirable. A perfect score of ME = 0 in fact does not exclude very large errors of opposite signs which cancel each other out.
Reply
We use ME as index of the overall bias and MRSE for the accuracy.

Ref#1
Page 13346, eq. (44): this equation is not correct. For a right normalization you should take sigma_SD out of the root square, otherwise the computed RMSE would not be dimensionless and could not be compared between the h-form and theta-form scenarios. This error casts doubt on the results presented in Table 3 and discussed later on the in the manuscript.
Reply
This is a banal editing error, we are sorry for that. Values in Table 3 are correct.

Ref#1
Page 13347, lines 10-11: in my opinion this is a critical issue. Could it be related to the fact that the Crank–Nicolson approximate solution can contain spurious oscillations in certain conditions? The backward Euler method is both stable and immune to oscillations but of course must be coupled with a nonlinear KF-extension such as, e.g., the ensemble Kalman filter.
Reply
We checked for numerical errors by comparing the results obtained with the Crank-Nicolson with those obtained with the backward Euler method. We also reduced the time step in the executions. The stability of the CN numerical solution is not an issue. For example, difficulties may arise in the initial stages of the assimilation process when dealing with marked differences between the estimated states and the observations and with a set of guess parameters that indicates a wrong retrieving track. It should be also seen in the context of a simulation, where the parameter adaptability is constrained by the parameter covariance.

Ref#1
Page 13347, lines 16-23: have you tried a simpler log-transformation of the parameters? It would probably suit better the hydraulic conductivity and the range of search would not be limited between two values, a characteristic that could help when no prior information are available.
Reply
The sigmoidal transformation is for us an important point of the proposed assimilation algorithm.

Yes, we (unsuccessfully) tried a log-transformation of the parameters. Given the very high correlation between them, we commonly found divergent solutions. This problem is not solved by just constraining the parametric space: in this case the covariance indefinitely increases and the solution remains at the extremes. The advantage of the sigmoidal transformation is that we constrain the domain of the parameters by means of a function having a domain equal to [-∞, +∞]. This approach guarantees in principle the possibility to find the right track toward a convergent solution.
We employed relatively large ranges of variability for the parameters and the bounds have been chosen based on physical considerations.

Ref#1
Page 13347, line 24: the covariance matrices should be chosen on the basis of physical considerations and not be tuned to ensure the convergence of the method.
Reply
Here we refer to the covariances linked to the parameters (or more exactly to the correction terms, according to the sigmoidal transformation). The choice of these initial covariances mediates not only physical, but also practical grounds. Nelson (2000), dealing with a Dual EKF application, reports: "*a main conclusion* [concerning the initialization of covariances] *is that too large a value of the initial parameter covariance can sometimes prevent the dual EKF from converging.*"
The assessment of the influence of the initial covariances was part of the study.

Ref#1
Page 13348, lines 7-8: on the other hand, it should be mentioned that, contrary to the h-based form, the theta-based equation does not allow solving problems involving also the saturated zone.
Reply
We already acknowledged this in the first part of our study. We can mention this aspect here as well.

Ref#1
Page 13349, lines 14-15: I would rather say that Ks is not identifiable, as it diverges even when the initial guess is close to the true value.
Reply
We discussed this point in the paper (see page 13356, lines 18-25):
"The assimilation of near surface soil moisture observations recalls some considerations about the sensitivity to the VGM parameters, at least when the system is initialized with wet conditions. The indentifiability of parameter is markedly higher than that of n, particularly when using pressure head as retrieving variable. Instead the identifiability of the saturated hydraulic conductivity is in all cases very poor. This fact, joined with the strong correlation observed between retrieved n and Ks, suggests the opportunity to employ other analytical models, representing the hydraulic conductivity decoupled from the retention function."

Ref#1
Page 13349, lines 25-29: perhaps it depends on the quality of the figure (it is very hard to make out the different lines), but I cannot see a clear difference between prior n > 2 and < 2. In particular, scenarios with prior n = 2.6 seem to converge no differently from the other ones. Slight differences can only be discerned in the theta-theta retrieving modes.

Reply

Really our arguments give a biased message, and should be better explained. The differences between initial n values >2 and < 2 using the *h-h* mode, concern principally the stability of the retrieving algorithm, with the former (n>2) being more vulnerable to this issue.

In principle, stability can affect also the simulations with initial n<2, when the parameter stably adopts a value higher than that threshold, during the "erratic" first few updates. The randomness level of these first stages is chiefly controlled by the initialization of the parameter covariances, a complex issue discussed in section 5.5.

The statements of *lines 25-29* are not only the result of the analysis of Fig 1 for the *h-h* mode (where one can notice that for initial n=1.6 [S1(○), S2(□)] the convergence track is much smoother and regular than for initial n>2), but also of several complementary analyses, as indicated in the next paragraph.

We reckon that the message is also affected by the sentence "*The convergence toward the true n is more delayed as compared with* α*"*, which is contextually inappropriate. This statement, attributable to both the *h-h* and the θ-θ modes, breaks the continuity of the discussion between the previous sentences and the following sentence and paragraphs.

We propose to modify the paragraph accordingly.

The quality of the Fig. 2 will certainly improve when the figure is printed on a full A4 paper, as it should be. Unfortunately, the HESSD editing service squeezes the figures in half A4.

Ref#1

Page 13350, lines 7-14: in view of the previous point, this discussion can be removed altogether, as well as Figure 3 and lines 1-8 at page 13351.

Reply

As sustained in our reply, we think these lines and the figure are important to understand the different behaviours obtained with the *h*- and the θ-forms.

Ref#1

Page 13350, lines 26-29: again, this is very subtle and, to tell the truth, it seems to me that the contrary occurs (see previous point).

Reply

Here we referred just to the first assimilations, where we observed that, even for n=2.6, the updating consistently orientates toward the convergent solution. We recognize that the distinction between the cases n>2 and n<2 is rather subjective. We propose to modify the sentence as follows: "*As an opposite trend with respect to the h−h retrieving mode, it is possible to appreciate that the indentifiability improves during the initial stage of the simulated process, characterised by high soil water content values.*

Ref#1

Page 13351, lines 9-14: I do not agree that these results are encouraging. Neither the results about Ks, which is of fundamental importance and cannot be retrieved, nor those about n and alpha are conclusive. It seems that in all cases the solution converges to values that are not far away from the initial guess, so a few questions remain. What happens if you start from prior guesses that are further away from the truth? Is the solution found by the method better than the prior? In other words, are the errors associated to a posteriori simulations run with the retrieved parameters smaller than the errors computed by simulations run with the prior parameters (open loop)?

Reply

We suspect that the opinion of the referee is influenced by the scale of the figures, where all the examined cases are considered. Please note, from Table 2, that the limit values of our parameters cover practically the overall spectrum of values reported by Carsel and Parrish (1998) for 12 major soil textural groups, except (but only partially) for the sandy soils.
Looking at Figure 5 representing the state profiles, one can conclude that the retrieving algorithm is efficient from a strict functional perspective, provided that the states are retrieved with high accuracy, particularly in the θ-θ mode, but also in *h*-*h* mode, except for two initial parameter sets, as explained in the manuscript. Also note that we did not represent the open loop profiles in Figure 5 just to keep the figures to a suitable scale. The open loops profiles are indeed completely out the range considered.
Thus, given the good state retrieving performances, we believe that the issues experienced in parameter retrieving are to be attributed to the high correlation between the van Genuchten parameters, as reported in numerous previous studies, which irremediably affects the overall identifiably, and not surprisingly, particularly that of K_s.
Another main factor concerns to the limited *observability*, associated to the very narrow range covered by the state variables in the considered experiment.
This drawback is reflected in the manuscript (p. 13349, L.10-13): "*Several authors evidenced the limitations for a successful estimation of VGM parameters, as imposed by the narrow variability of naturally occurring boundary conditions (Scharnagl et al., 2011; Vrugt et al., 2001, 2002). A wide range of soil moisture states in required to reliably constraining the soil hydraulic functions*".
Vrugt et al. (2003) states that *"experiments that yield a wide range of water contents or pressure heads are beneficial for parameter estimation studies, since the measurements then contain independent information for most of the parameters. This increases the identifiability of the parameters and enhances the likelihood of uniqueness of the final parameter estimates*." He also shows that the maximum sensitivity of the parameters α and n occurs at high pressure head values in fine-textured soil. According to his work, good indentifiability of *n* in clay soil demands pressure values well beyond -10^4 cm. In our case we worked with a clay loam soil, covering a limited range of pressure heads (see Fig. 1 in the manuscript).
Probably the use of a single metrics conspires also against the wished identifiability, as reflected by Vrugt et al. (2012). Nevertheless, even the retrieving pattern of K_s, for which we recognize that the identifiability is poor, responds to a logical behaviour, as indicates the very good agreement between the evolving parameter cross-covariance and that reported in several works (e.g. Romano and Santini, 1999; van Dam, 2000). In the companion paper (Medina et al., 2012) we provide some elements about this issue.

Ref#1

Page 13351, lines 21-23: this is very contradictory. It may be that the error on RMSE (see previous point at Page 13346, eq. (44)) affects these results and thus leads to ambiguous conclusions. Please double-check the RMSE.

Reply

Effectively, the current writing provides a contradictory message. Sorry for this. We propose to change the statement as follows:
"The soil moisture retrieval clearly outperforms the analogous pressure head retrieving using the lowest temporal and spatial resolution of the observations. The evolving pressure head profiles S4 and S5 using AF=1/5 days−1 are permanently biased. This result reflects the abnormal pattern of the evolving retrieved parameters associated with these two sets (Fig. 4a), both characterized by an initial guess n>2. Nevertheless, as shown later, the average RSME of the convergent pressure head profiles is generally lower than the homologous using soil moistures."

Ref#1

Page 13352, lines 13-15: this is somewhat surprising. Can you explain why a higher assimilation frequency would yield worse results?

Reply

It is certainly a not expected, although perfectly possible, result. This result shows that, for this experiment, the retrieving process is not particularly sensible to the assimilation frequency, at least within examined range of frequency values. This is most probably related to the sampled observations in each case, being in general different, and consequently with dissimilar impact on the overall statistics. Note that this trend changes with the increasing OD, i.e., when more pieces of information are available.

Ref#1

Page 13352, lines 20-22: again, this statement seems to contradict the consideration at page 13351, line 21.

Reply

The statement is again valid to those stable (convergent) *h-h* solutions, but it is not clear in our text. Sorry for this. We propose to modify it as follows:

Once the stability of the h-h solution is ensured, the convergence of the predicted pressure head profiles to the SD ones is also clearly faster than the predicted soil moisture profiles.

Ref#1

Page 13354, lines 1-6: much more details are needed here. Stating "the unscented algorithm is also employed for the statistical linearization of the now nonlinear operator H, similarly to what is done for retrieving the parameters" is not sufficient. How has this been done? What parameter values have been used? Rewriting section 2.1.2. could help to shed more light on this subject, too.

Page 13354, lines 10-14: this is one of the reasons for which the ensemble Kalman filter is more popular than EKF for this kind of applications.

Reply

These comments will be taken into consideration in the revised manuscript.

Ref#1

Page 13355, lines 3-15: much more details are needed here. The reader might want to reproduce the results and, for doing so, need to know exactly what values have been used in each scenario. Suggest adding a table that includes all the parameter values used for each scenario. Besides, if the algorithm is so dependent on the choice of the matrices, it does not seem to be really robust. Could you please comment on that?

Reply

We will follow your suggestions in the reviewed manuscript.

Certainly the implementation of a *dual* (or a *joint*) exercise for parameter-state estimation demands more caution, as compared with a standard KF approach, particularly for what concerns the initialization of the covariances, not only of the parameters but even of the states. Liu and Gupta reports: a joint approach could produce "*process unstable and intractable because of complex interactions between states and parameters in nonlinear dynamic systems (Todini, 1978a, 1978b). In addition, since parameters generally vary much more slowly than the system states, unstable problems may also result from the fact that both model states and parameters are updated at each observation time step in this method. This same argument may apply to the dual state-parameter estimation methods presented by Moradkhani et al. (2005a, 2005b).*" This can be seen as the price to be paid for a more accurate result.

According to our results, the retrieving algorithm using the *h-h* mode was sensible to the choice of the covariance matrices; instead the θ-θ counterpart was relatively easy to implement in this synthetic study (but also for a practical one, as shown in the companion paper Medina et al. 2012). Nevertheless, as stated above, a significant weight on the performance of the overall algorithm lays on the constitutive relationships appearing in the Richards equation. We believe further attempts should be focussed to the evaluation of some alternative analytical expressions, other than the van Genuchten model, possibly the hydraulic function decoupled from the water retention function.

Ref#1

Page 13356: In view of all the points above, I would recommend the conclusions be rewritten. The dual Kalman filter approach seems to have more cons than pros and the implementation of the UKF does not seem so simple. After double-checking the results, the Authors could reconsider some of the statements on the sensitivity to the VGM parameters and the comparison between system state retrieval in the h-based and theta-based scenarios. Finally, the final considerations concerning "the convenience of retrieving state variable of the same type of the observation variable" cannot be generalized. As mentioned earlier, the EnKF has been demonstrated to work fine with nonlinear observation models as well as with linear ones.

Ref#1

We agree with the Referee. We will account for these considerations in the revised manuscript.

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