Kalman filters for assimilating near-surface observations in the Richards equation – Part 3: Retrieving states and parameters from laboratory evaporation experiments
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Reply to Referee#I

We thank Referee#1 for the favourable appreciation of our work. Below we provide our replies to the Referee comments.

Ref#1

I would like the authors to explain more clearly why the fact of considering a Crank-Nicolson numerical scheme makes the Richards equation more linear and therefore avoids the need for an Extended Kalman Filter. An explanation has probably been given in the previous parts of this paper but it would be useful to have it here as well.

Reply

We will provide more information about the Crank-Nicolson numerical scheme, as applied to the Richards equation.

The Crank–Nicolson method is a finite difference method which reduces the partial differential equations into a set of discrete linear equations implicit in time.

The Richards equation, i.e., the governing soil water flow equation in its stochastic form, is:

$$C(h)\frac{\partial h}{\partial t}=\frac{\partial\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]}{\partial z}+v(t) \qquad \text{(c\#2.1)}$$

where $C(h)=\partial\theta/\partial h$ [1/L] represents the specific water capacity of the soil at pressure head h obtained by differentiating the soil water retention function $\theta(h)$, whereas $K(h)$ [L/T] represents the unsaturated hydraulic conductivity function. The functions $\theta(h)$ and $K(h)$ are described by the following non-hysteretic van Genuchten-Mualem (VGM; van Genuchten, 1980) relations, widely used in soil hydrology:

$$\theta(h)=\theta_r+(\theta_s-\theta_r)\left(1+|\alpha h|^n\right)^{-m} \qquad (28)$$

$$K(\theta)=K_s S_e^{\lambda}\left[1-\left(1-S_e^{1/m}\right)^m\right]^2 \qquad (29)$$

The corresponding discrete form of Eq. (c#2.1) according to the CN differential scheme for node i at time-step k+1 is for i=2,…,N-1:

$$\left(\frac{-K_k^{i-1/2}}{2\Delta z^i\Delta z^u};\frac{C_k^i}{\Delta t_k}+\frac{\frac{K_k^{i-1/2}}{\Delta z^u}+\frac{K_k^{i+1/2}}{\Delta z^l}}{2\Delta z^i};\frac{-K_k^{i+1/2}}{2\Delta z^i\Delta z^l}\right)\begin{pmatrix}h_{k+1}^{i-1}\\h_{k+1}^{i}\\h_{k+1}^{i+1}\end{pmatrix}=\left(\frac{K_k^{i-1/2}}{2\Delta z^i\Delta z^u};\frac{C_k^i}{\Delta t_k}-\frac{\frac{K_k^{i-1/2}}{\Delta z^u}+\frac{K_k^{i+1/2}}{\Delta z^l}}{2\Delta z^i};\frac{K_k^{i+1/2}}{2\Delta z^i\Delta z^l}\right)\begin{pmatrix}h_k^{i-1}\\h_k^{i}\\h_k^{i+1}\end{pmatrix}+\frac{K_k^{i-1}-K_k^{i+1}}{2\Delta z^i}+v_k^i \qquad \text{(c\#2.2)}$$

For nodes i=1 and i=N the discrete forms at time-step k+1 are:

$$\left(\frac{C_k^1}{\Delta t_k}+\frac{K_k^{1\frac{1}{2}}}{2\Delta z^1\Delta z^l};\frac{-K_k^{1\frac{1}{2}}}{\Delta z^1\Delta z^l}\right)\begin{pmatrix}h_{k+1}^1\\h_{k+1}^2\end{pmatrix}=\left(\frac{C_k^1}{\Delta t_k}-\frac{K_k^{1\frac{1}{2}}}{2\Delta z^1\Delta z^l};\frac{K_k^{1\frac{1}{2}}}{\Delta z^1\Delta z^l}\right)\begin{pmatrix}h_k^1\\h_k^2\end{pmatrix}+\frac{q_{top}^1-K_k^{1\frac{1}{2}}}{\Delta z^1}+v_k^1 \qquad \text{(c\#2.3)}$$

$$\left(\frac{-K_k^{N-1/2}}{\Delta z^N\Delta z^u};\frac{C_k^N}{\Delta t_k}+\frac{K_k^{N-1/2}}{2\Delta z^N\Delta z^u}\right)\begin{pmatrix}h_{k+1}^{N-1}\\h_{k+1}^{N}\end{pmatrix}=\left(\frac{K_k^{N-1/2}}{2\Delta z^N\Delta z^u};\frac{C_k^N}{\Delta t_k}-\frac{K_k^{N-1/2}}{2\Delta z^N\Delta z^u}\right)\begin{pmatrix}h_k^{N-1}\\h_k^{N}\end{pmatrix}+\frac{K_k^{N-1/2}-q^N}{\Delta z^N}+v_k^N \qquad \text{(c\#2.4)}$$

The forecasting equation of the system state $\boldsymbol{x}_k$, coinciding with the matric pressure head ($x_k^i = h_k^i$), can be obtained by combining the discrete equations written for all N nodes in the following linear state-space form:

$$\hat{\boldsymbol{x}}_{k+1}^- = \mathbf{A}_k^{-1}\mathbf{B}_k\boldsymbol{x}_k + \mathbf{A}_k^{-1}\boldsymbol{g}_k + \mathbf{A}_k^{-1}\boldsymbol{v}_k \qquad \text{(c\#2.5)}$$

where $\mathbf{A}_k$ is the tri-diagonal matrix obtained by assembling the terms in the first parenthesis on the right hand-side of Eqs. (c#2.2-2.4), $\mathbf{B}_k$ is the tri-diagonal matrix obtained by assembling the terms in the first parenthesis on the left hand-side of Eqs. (c#2.2-2.4). The term $\boldsymbol{g}_k$ is a vector obtained by assembling the source terms on the right hand-side of Eqs. (c#2.2-2.4) which are independent from the process noise.

Ref#1

I found that too many results are presented, in particular the fact of having chosen a set of 6 initial parameters (S1 to S6) makes Table 4 and Figures 2 to 12 (except Figure 11) difficult to read and does not bring a lot of additional information (slower convergence when initial parameters are farther from the optimal solution). I suggest to simply keep one set of initial parameters and maybe to have a paragraph discussing the sensitivity of the results to the choice of initial parameters.

Reply

We pondered that possibility in a previous version of the manuscript, but the overall balance of simplifying the figures and supporting the results only by the discussion was clearly discouraging. The choice of the initial set of parameters has an important impact on the retrieving process. Therefore we would prefer to keep the figures as they are.

Ref#1

Similarly, considering 3 observation depths is not very useful: indeed the 1 cm layer is shown to be less informative about the deeper layers than the 2 cm layer. Even though the 12 cm depth is providing some kind of upper bound for the behaviour of the assimilation, it is an unrealistic set-up in the context of remote sensing information. Results shown with OD=2cm are convincing enough.

Reply

We also believe that showing the results for different assimilation depths is important for a comprehensive evaluation of the assimilation algorithm. The observation depth of OD=12 cm, which is the same as assimilating the entire profile, has been included as benchmark performance for OD=1 cm and OD=2 cm in the parameter identification.

Ref#1

Can the authors provide an explanation about the negative Kalman gain coefficient K12,1? Is there a decoupling in terms of behaviour between the first layer and the soil column below ? At least such negative value explains why using an observations at OD=1cm is not so useful.

Reply

We believe that the observed pattern is strongly linked to the initial condition, i.e. a constant soil moisture profile at the left (the drier part) of the actual profile.

If state and observation variables are the same, the matrix **H**, having 2 rows and 12 columns, adopts the form:

$$\mathbf{H}=\begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \end{pmatrix}$$

In this case the sign of the Kalman gain coefficients is intrinsically linked to those of the state covariance considering the relationship:

$$\mathbf{K}_k = E\left[\left(\boldsymbol{x}_k - \hat{\boldsymbol{x}}_k^-\right)\left(\boldsymbol{y}_k - \hat{\boldsymbol{y}}_k^-\right)^T\right]E\left[\left(\boldsymbol{y}_k - \hat{\boldsymbol{y}}_k^-\right)\left(\boldsymbol{y}_k - \hat{\boldsymbol{y}}_k^-\right)^T\right]^{-1} = \mathbf{P}_{x\tilde{y},k}^-\left[\mathbf{P}_{\tilde{y},k}^-\right]^{-1} = \mathbf{P}_{\mathbf{x}_k}^-\mathbf{H}_k^T\left(\mathbf{H}_k\mathbf{P}_{\mathbf{x}_k}^-\mathbf{H}_k^T + \mathbf{R}_k\right)^{-1}$$

The inverse of $\mathbf{P}_{\tilde{y},k}^{-}$ does not modify the sign of the coefficients of $\mathbf{P}_{\mathbf{x}_k}^{-}\mathbf{H}_k^T$.

Hence, a negative $K_{12,1}$ manifests the negative cross-covariance between the states 1 and 12 ($P_{12,1}$). The analogous reasoning is also valid for $K_{12,2}$.

Under the adopted experimental settings the guess states transit from a uniform matric potential profile to a distribution close to a uniform head profile. It means that the bottom nodes move toward a wetter range, while the evaporative process drives the opposite trend on the top node. The zero flux condition at the bottom profile favours the relatively large duration of this phase of the process. During these stages the correlation between the first and the bottom nodes is markedly negative, which determines a negative sign of $K_{12,1}$. According to Figure 11, this phase lasts approximately one day for GA3 and two days for GB1.

When this trend changes, with the bottom nodes also moving to a drier range (although much more slowly than the top node), the estimated $P_{12,1}$ increases, i.e., it gets less negative values.

Ref#1

Would there be an interest for a combined assimilation for state and parameter retrievals, instead of the parallel assimilations proposed in the paper?

Reply

A joint assimilation scheme can be an alternative to the dual assimilation scheme herein adopted. However, we would be forced to implement the algorithm with a single non-standard Kalman filter (e.g., the unscented Kalman Filter or the Ensemble Kalman Filter). By using separate filters for states and parameters can take advantage of the marked differences in the variability patterns of these two types of variable.

Liu and Gupta (2007) report: *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.*"

These issues (the complex interactions between retrieved states and parameters and the marked differences in their variability patterns) are even more relevant under the adopted (yet necessary) strategy involving the parameter transformation with the help of a sigmoidal function.

References

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