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Obtaining soil hydraulic parameters from soil water content data assimilation under different climatic/soil conditions

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ABSTRACT

Obtaining reliable soil hydraulic properties is essential for correct simulations of soil water content (SWC), which is a key variable in countless applications such as agricultural management, soil remediation, aquifer protection, etc. Soil hydraulic properties can be measured in the laboratory; however, the procedures are laborious and costly, and may provide estimates different from those observed in the field. An alternative approach is to obtain soil hydraulic properties using a soil water flow model in conjunction with SWC monitoring data. The goal of the present study was to analyze the efficiency of obtaining hydraulic properties utilizing data assimilation (DA) based on the Ensemble Kalman Filter method. Two soil textures in homogeneous soil profiles, and four climatic conditions were considered; observations of soil moisture data were synthetically generated using HYDRUS-1D and subsequently perturbed by the application of the conditional multivariate normal distribution. When observed SWC varied in relatively narrow range as a consequence of the forcing imposed by dry climate atmospheric boundary conditions, data assimilation provided sets of properties that led to good Richards model performance, with the RMSE below 0.02 and/or R^2 above 0.8 after a period of just 100 days and above 0.98 after a period of three years in all climate/soil conditions. However, the closeness of parameters from DA to the parameters used to generate the synthetic data depended on weather conditions and soil properties. One year was adequate to obtain reliable soil hydraulic properties with data assimilation.

1. Introduction

Soil water plays an essential role in the global water cycle: it has an important impact on weather, climate and energy fluxes at the land surface, drives agricultural management, and gives shape to the organization of ecosystems. The role of soil water is extremely significant in arid and semiarid regions, where water scarcity has an important impact on plant production (Vereecken et al., 2008) and soil salinization (Ritzema, 2016), and overall imposes constraints to society development (Lattemann and Höpner, 2008). A wide variety of activities rely on estimates of changes in soil water content (SWC) under various environmental and anthropogenic controls. Such estimates employ soil hydraulic parameters quantifying the soils' ability to hold and transmit water.

Measuring soil hydraulic properties in the laboratory is labor- and time-consuming, and may provide results different from those observed in the field due to differences in the soil volume involved, soil disturbance during sampling, short circuit flow through macropores or along core wall in lab, continuity in the soil profile versus depth, etc. (Ramos et al., 2006; Rezaei et al., 2016). An important viable alternative is to derive soil hydraulic properties from soil water flow modelling in conjunction with SWC monitoring. One methodology available for that purpose is data assimilation (DA).

Data assimilation methods improve the model performance by integrating observed data (i.e., system states) into the modelling process in order to correct the model predictions (Evensen, 2009; Plaza et al., 2012). Data assimilation was initially applied to atmospheric and oceanic system modelling (Lahoz et al., 2010), where it has become a common approach. The DA has a substantial history of applications in soil water modelling (Or and Hanks, 1992; Pan et al., 2012; Vereecken et al., 2008). It was originally used with observed states as initial conditions, and updated in successive runs with new observation states, Chirico et al. (2014) compared different Kalman filtering alternatives. Later on, the DA has been applied to jointly update model states and soil hydraulic parameters (Li and Ren, 2011; Medina et al., 2014; Montzka et al., 2011; Moradkhani et al., 2005b; Song et al., 2014; Vrugt et al., 2005a; Vrugt et al., 2005b).

The Ensemble Kalman Filter (EnKF) is one of the most widely used

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DA methods (Moradkhani et al., 2005b; Zhang et al., 2016). It is a sequential Monte Carlo-based method, first introduced by Evensen (1994) and later clarified by Burgers et al. (1998). In brief, an ensemble of models is randomly generated, then propagated in time to the to the next update event. For each update event, a state error covariance matrix is calculated from the state values simulated by the different ensemble members before the update (a priori). This covariance state matrix is used jointly with the covariance matrix of observations at the same time to obtain a new set of model states (the posterior). The EnKF has been proven to be an efficient approach to correct the Richards equation-based soil flow modelling results (Das and Mohanty, 2006). Vereecken et al. (2008) and Vrugt et al. (2005a) noted that the conceptual simplicity, relative ease of implementation and computational efficiency make the EnKF method an attractive option for sequential data assimilation in vadose zone hydrology. The assumption of a Gaussian distribution in errors that EnKF does cannot always be accepted in hydrological modelling, and new data assimilation alternatives such as particle filter, firstly introduce in hydrology by Moradkhani et al. (2005a), avoid the requirement of error Gaussian distribution; toward that end, the Markov Chain Monte Carlo method (Moradkhani et al., 2012; Vrugt et al., 2013) appears to be a powerful technique.

Li and Ren (2011) demonstrated the efficiency of the DA in joint state–parameter estimations for soil water dynamics in experiments with constant boundary conditions compared to standard calibration. These authors researched the applicability of the EnKF to assimilate data from infiltration and drainage experiments. Erdal et al. (2012) demonstrated applicability of EnKF to the dataset collected from lysimeters with soil under wheat over the growing season. Erdal et al. (2014) showed that the EnKF could result in reasonable estimates of effective hydraulic properties even if the model has structural errors. Li and Ren (2011) identified factors affecting results of the soil water data assimilation with EnKF, including the initial estimate selection, the ensemble size, the observation error and the model error, the assimilation interval, the water regime, and the variability of the estimated parameters. Other factors of DA performance are model simulation time step, the number of parameter for estimation (degree of freedom in inverse modelling), and the quality of the assimilated data. The role of these factors was researched by Li and Ren (2011) for DA from one-directional flow and constant boundary condition experiments. The effect of the initial values of parameters on their temporal evolution has not been considered in the present study and it remains to be seen and addressed in future studies how the errors in initial parameter values manifest themselves in different climatic and soil conditions.

The objective of this work was to analyze the efficiency of the joint soil water state – parameter estimation under contrasting climatic conditions and soil types to infer soil hydraulic properties. Besides, the study aims to improve knowledge about how long should be the observation period of time to be able to reproduce the field soil water dynamics with the model.

2. Materials and methods

2.1. Water flow modelling

Water flow modelling was conducted with the HYDRUS-1D software (Šimůnek et al., 2009) numerical solution. The variably saturated water flow was modelled according to Richards equation (Richards, 1931):

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left(K(h)\cdot\left(\frac{\partial h}{\partial z} + 1\right)\right) - S(h) \tag{1}$$

where θ is volumetric water content [$L^3 \cdot L^{-3}$]; t time [T]; z is the vertical coordinate [L]; $K(\theta)$ is the soil unsaturated hydraulic conductivity [$L\cdot T^{-1}$]; h is the soil water pressure head [L]; and $S(h)$ is the sink term that represents water uptake by plants [$L^3 \cdot L^{-3} \cdot T^{-1}$]. The hydraulic properties were defined with the van Genuchten-Mualem constitutive relationships (Mualem, 1976; van Genuchten, 1980):

$$\theta(h) = \begin{cases} \theta_r + (\theta_s - \theta_r)\cdot[1 + |\alpha\cdot h|^n]^{-(1-1/n)} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \tag{2}$$

$$K(h) = K_s \cdot S_e^l (1 - (1 - S_e^{n/(n-1)})^{1-1/n})^2 \tag{3}$$

where S_e is the effective saturation:

$$S_e = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \tag{4}$$

and θ_s the saturated water content [$L^3 \cdot L^{-3}$]; θ_r is the residual water content [$L^3 \cdot L^{-3}$]; K_s is the saturated hydraulic conductivity [$L\cdot T^{-1}$]; and α [L^{-1}], n [−], and l [−] are empirical coefficients that determine the shape of the hydraulic functions. The value of $l = 0.5$ is commonly assumed, based on Mualem (1976).

Atmospheric boundary conditions were defined on a daily basis. Maximum computational time step was set to one day, but smaller computational time steps occurred to assure convergence.

2.2. Data assimilation with EnKF

Data assimilation was conducted using the Ensemble Kalman Filter method with a state augmentation approach. Assume the ensemble consists of N models that predict s state variables (among them, m of these variables are observed in the field) and the number of model parameters to be updated are p. After each time step, values of s states variables from the N models of the ensemble are collected in a matrix $\mathbf{X}$ (s,N). The matrix $\mathbf{Y}(p,N)$ is the parameter ensemble and collects values of p model parameters which are updated in each time step. In the state augmentation approach, both state and parameter matrices are combined into a single one, the augmented state matrix $\mathbf{Z}(p + s,N)$ being as follows:

$$\mathbf{Z}_t = \begin{bmatrix} \mathbf{Y}_t \\ \mathbf{X}_t \end{bmatrix} \tag{5}$$

In each updating time, a new augmented matrix is obtained as follows:

$$\mathbf{Z}_t^+ = \mathbf{Z}_t^- + \mathbf{K}_t(\mathbf{D}_t - \mathbf{H}\cdot\mathbf{X}_t) \tag{6}$$

where $\mathbf{Z}_t^-$ and $\mathbf{Z}_t^+$ are the prior and posterior augmented matrices at time t, respectively and $\mathbf{K}_t$ is the gain Kalman matrix ($p + s$,m) in time t. Matrix $\mathbf{D}_t(m,N)$ is created adding to the observed values a white noise based on the data variances and covariance of observed values; it stores N different replicates of m soil moisture observations at time t. $\mathbf{H}(m,s)$ is the observation matrix that relates observations and simulated states; if observation and model states are equal, then $\mathbf{H}$ becomes the identity matrix; when, as in the present study, observation and model states are both volumetric water content but there are more model states than observations, $\mathbf{H}$ becomes a rectangular matrix with 1 and 0, that 'picks up' the model states used in the updating process.

The gain matrix relates the variability of modelling results and variability in the data. It is computed on each updating time as:

$$\mathbf{K}_t = \mathbf{C}_{YX-XX}\cdot\mathbf{H}^T\cdot(\mathbf{H}\cdot\mathbf{C}_{XX}\cdot\mathbf{H}^T + \mathbf{R})^{-1} \tag{7}$$

where $\mathbf{C}_{XX}(s,s)$ is the covariance matrix of the state simulations; $\mathbf{R}(m,m)$ is the covariance matrix of observed values; and $\mathbf{C}_{YX-XX}(p + s,s)$ is the covariance matrix tying the variability of the augmented states and the states simulations. The complete covariance matrix, $\mathbf{C}_t(p + s,p + s)$, is estimated from the ensemble (N units) of the augmented parameter-state matrix $\mathbf{Z}(p + s,N)$, and it is defined as:

$$\mathbf{C}_t = \begin{pmatrix} \mathbf{C}_{YY} & \mathbf{C}_{YX} \\ \mathbf{C}_{XY} & \mathbf{C}_{XX} \end{pmatrix} \tag{8}$$

where the $\mathbf{C}_{YY}(p,p)$ refers to covariances between parameters; $\mathbf{C}_{XX}$ to