Comparison of ensemble data assimilation methods for the estimation of time-varying soil hydraulic parameters

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ABSTRACT

The hydraulic properties of the soil top layer may change during the growth period due to various factors such as wetting and drying cycles, tillage practices, and crop root growth. In this study, the potential of the assimilation method to estimate time-varying soil hydraulic parameters is explored. Four assimilation schemes, including the simultaneous update state augmentation method, the partitioned update state augmentation method, the simultaneous update parameter correction method, and the partitioned update parameter correction method, are compared. The performance of four assimilation schemes on parameter estimations and soil moisture simulations is tested first using the synthetic case. The influence of initial parameter values and a parameter update order on assimilation is also analyzed. Finally, the partitioned update parameter correction method is applied to a real case involving a field drip irrigation experiment. The results show that when the analyzed parameter has either a periodical or a linear variation, there is a time lag between the assimilation value and the true value. The assimilation method can respond immediately to an abrupt change of the parameter value. Using the simultaneous update method leads to an obvious parameter correlation problem. In contrast, the partitioned update method can relieve the parameter correlation problems, thereby improving the accuracy of parameter estimations and pressure head simulations. However, when the initial values of the parameters deviate from their true values to a certain extent, the partitioned update method cannot obtain accurate parameter estimations. Compared with the partitioned update state augmentation method, the partitioned update parameter correction method is not sensitive to the parameter update order. The partitioned update parameter correction method has higher computational efficiency and assimilation stability, and it can obtain more accurate parameter estimations and soil moisture predictions in comparison with the traditional state augmentation method. The partitioned update parameter correction method provides an assimilation tool for improving the predictions of soil moisture by considering the time-varying parameters.

1. Introduction

Influenced by wetting and drying cycles (Mubarak et al., 2009), tillage practices (Mohanty et al., 1994; Cameira et al., 2003), and crop root growth (Rasse et al., 2000; Iqbal et al., 2005), the hydraulic properties of the soil top layer can change during the growth period. Using time-varying soil hydraulic parameters can improve the accuracy of soil moisture simulations (Schwen et al., 2011). However, only a small number of studies have focused on soil moisture modeling for time-varying parameters (Or et al., 2000; Xu and Mermoud, 2003; Schwen et al., 2011).

In order to obtain time-varying soil hydraulic parameters, the common practice is to conduct field infiltration experiments or take measurements on soil samples in the laboratory at intervals during the simulating period (Xu and Mermoud, 2003; Mubarak et al., 2009; Schwen et al., 2011), which is labor-intensive and time-consuming. Also, the parameters obtained in the laboratory may not be suitable for field applications due to the scale effect. Inverse modeling provides an alternative method and has been widely used to estimate soil hydraulic parameters (Pan and Wu, 1998; Abbaspour et al., 2001; Lambot et al., 2011).

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et al., 2002; Li and Ren, 2011; Brandhorst et al., 2017).
There are mainly three kinds of inverse methods for estimating time-varying parameters. The first approach considers a functional form of the time-varying parameter (Westra et al., 2014; Jeremiah et al., 2013). The second approach divides observation data into several consecutive time intervals and calibrates the model parameters for each interval separately (Thirel et al., 2015; Merz et al., 2011; Gharari et al., 2013). However, artificially selecting the functional form or dividing the time intervals still requires scientific judgment, which is often difficult (Pathiraja et al., 2016). Finally, the third approach, i.e., assimilation method, updates parameters automatically when observation data is available. Several studies have investigated the potential of data assimilation methods to estimate time-varying parameters. Pathiraja et al. (2016) proposed a multi-layer ensemble Kalman filter (EnKF) method and a local linearization method to estimate the parameters of a conceptual hydrological model PDM (Moore, 2007). However, the multi-layer EnKF method requires estimation of the hyperparameter in addition to the model parameters, thus increasing the number of parameters to be estimated. The local linearization method assumes that there is a linear relationship between the parameters at the current time and the previous time. Hence, it cannot deal with the situation when the parameter value has abrupt changes. Deng et al. (2016) and Xiong et al. (2019) used the constrained EnKF method to estimate the parameters of the water balance model TWBM (Xiong and Guo, 1999). The results show that the constrained EnKF method can obtain accurate parameter estimations, but there are time lags between the estimated value and its true value when the parameter has a periodical variation. Smith et al. (2008) proposed a technique based on a particle filter to evaluate the model’s structural inadequacy. In this method, the parameters were treated as evolving in time. Vrugt et al. (2013) and Salamon and Feyen (2009) also tested the temporal evolution of model parameters based on the particle filter method. However, the particle filter method is computationally very intensive.

Most of the existing studies estimating time-varying parameters using the assimilation method involve the conceptual hydrological model. Since soil hydrodynamic models usually have strong nonlinear behavior, the assimilation method’s potential to estimate time-varying soil hydraulic parameters needs further testing. In addition, the state augmentation technique is usually used to estimate soil hydraulic properties within the EnKF method (Li and Ren, 2011; Shi et al., 2015; Bauer et al., 2016; Brandhorst et al., 2017; Wu and Margulis, 2011), in which parameters and state variables are included in a state vector and updated simultaneously. However, this technique’s disadvantage is that when the number of unknown model states and parameters is large, the degree of freedom for high-dimensional vectors increases, making the estimation unstable, especially in nonlinear dynamic models (Mordkhanli et al., 2005; Xie and Zhang, 2013). Xie and Zhang (2013) proposed a partitioned update scheme for state-parameter estimation based on the EnKF method, in which the parameter set is partitioned into several types according to their sensitivities, and each parameter type is updated in an individual loop of assimilation. Lei et al. (2019) proposed a parameter correction method based on the EnKF framework, in which the state vector consists of parameters to be estimated.

To the best of our knowledge, there exists no research on estimating time-varying parameters of a soil hydrodynamic model using the data assimilation method. The purpose of this study is to explore the potential of the assimilation method to estimate time-varying soil hydraulic parameters. We compare four assimilation schemes: the simultaneous update state augmentation method, the partitioned update state augmentation method, the simultaneous update parameter correction method, and the partitioned update parameter correction method. The remainder of this paper is organized as follows. In Section 2, the soil hydrodynamic model and the assimilation algorithm are introduced. Section 3 illustrates a synthetic case and a real case involving a drip irrigation experiment. Results and discussion are presented in Section 4. Finally, conclusions are summarized in Section 5.

2. Methodology

2.1. Soil hydrodynamic model

The soil moisture dynamics can be described using the Richards equation:

\[
\frac{\partial \theta}{\partial t} - \frac{\partial}{\partial x} \left(K \left( \frac{\partial h}{\partial x} + K_0 \right) \right) - S = 0
\]

where \( \theta \) is the volumetric moisture content \([L^3 L^{-3}]\), \( h \) is the pressure

<table>
<thead>
<tr>
<th>Parameter</th>
<th>1st layer</th>
<th>2nd layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta_1 ) (cm(^3) cm(^{-3}))</td>
<td>0.399</td>
<td>0.399</td>
</tr>
<tr>
<td>( \theta_2 ) (cm(^3) cm(^{-3}))</td>
<td>0.0001</td>
<td>0.0001</td>
</tr>
<tr>
<td>( K_0 ) (cm min(^{-1}))</td>
<td>0.0207</td>
<td>0.0315</td>
</tr>
<tr>
<td>( \alpha ) (cm(^{-1}))</td>
<td>0.0174</td>
<td>0.0139</td>
</tr>
<tr>
<td>( \sigma ) (-)</td>
<td>1.376</td>
<td>1.602</td>
</tr>
</tbody>
</table>

Note: adapted from Simůnek et al. (2012).

Fig. 1. The computational domain for the synthetic case (a) and the initial pressure head profile and positions of observation points (b). Filled circles represent observation points.

Adapted from Simůnek et al. (2012)
Table 2
Soil physical properties for the real case.

<table>
<thead>
<tr>
<th>Soil depths (cm)</th>
<th>Soil particle fraction (%)</th>
<th>Soil texture</th>
<th>Bulk density (g cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-20</td>
<td>12.18</td>
<td>Sand &gt; 0.05 mm</td>
<td>26.84</td>
</tr>
<tr>
<td>20-40</td>
<td>21.84</td>
<td>Silt 0.002-0.05</td>
<td>1.47</td>
</tr>
<tr>
<td>40-60</td>
<td>18.46</td>
<td>Clay &lt;0.002 mm</td>
<td>1.49</td>
</tr>
<tr>
<td>40-80</td>
<td>0.0638</td>
<td>Silt loam</td>
<td>20.06</td>
</tr>
<tr>
<td>60-120</td>
<td>0.0910</td>
<td>Silt loam</td>
<td>1.53</td>
</tr>
<tr>
<td>80-160</td>
<td>0.0250</td>
<td>Silt loam</td>
<td>1.47</td>
</tr>
</tbody>
</table>

Table 3
Growth stages of processing tomato.

<table>
<thead>
<tr>
<th>Growth stage</th>
<th>Initial</th>
<th>Development</th>
<th>Mid-season</th>
<th>Late season</th>
</tr>
</thead>
<tbody>
<tr>
<td>Day</td>
<td>1-26</td>
<td>27-43</td>
<td>44-83</td>
<td>84-104</td>
</tr>
</tbody>
</table>

Fig. 2. The computational domain, boundary conditions, and positions of observation points for the real case.

head [L], K is the unsaturated hydraulic conductivity [L T⁻¹], K₀ and KᵢCam are components of a dimensionless anisotropy tensor KᵢCam, xᵢ and xⱼ are the spatial coordinates [L], and S is the sink term accounting for root water uptake.

The unsaturated hydraulic conductivity function is determined using the van Genuchten-Mualem model (Mualem, 1976; van Genuchten, 1980):

\[ K(h) = K₀S^{[1 - (1 - S^n)]^2} \]  

where \( K₀ \) is the saturated hydraulic conductivity [L T⁻¹], \( S \) is the effective water saturation [-], \( S₀ \) and \( Sₐ \) are the residual and saturated water contents, respectively, \( Sₐ = 1.7 \cdot 10^{-3} \), \( n \) is the pore-size distribution index [-]. In this study, unsaturated water flow was simulated using the CHAIN_2D code, a DOS predecessor of the HYDRUS model (Simůnek et al., 2008).

2.2. Parameter estimation based on the assimilation method

The assimilation method for parameter estimation consists of a model operator, an observation operator, and an ensemble Kalman filter algorithm. The model operator is used to pass the state vector to the next moment, which can be expressed as follows:

\[ X^{i+1} = M X^i + η^{i+1} \]  

where \( X^i \) and \( X^{i+1} \) are state vectors at current and next time, respectively; \( i \) and \( i + 1 \) denote time indicators; \( M \) is the model operator; \( η^{i+1} \) is the model error vector that is independent white noise for the model operator, which is drawn from a normal distribution with zero mean and specified covariance \( Q^{i+1} \).

The observation operator constructs the mapping between the state vector and the observation vector, which can be written as:

\[ Y^{i+1} = H^{i+1} X^{i+1} + ε^{i+1} \]  

in which \( Y^{i+1} \) is the observation vector; \( H^{i+1} \) is the observation operator; \( ε^{i+1} \) is the observation error vector, which is also assumed to be independent white noise drawn from a normal distribution with zero mean and specified covariance \( Q^{i+1} \).

The EnKF algorithm is a Monte Carlo method, in which the initial ensemble member can be generated by adding a random disturbance to the initial state vector, which can be expressed as follows:

\[ X^0_j = X^0 + ζ_j \]  

where \( j \) indicates the \( j \)th member in the state vector; \( ζ_j \) is independent white noise, which follows a multi-normal distribution with zero mean and specified covariance \( R \).

In the implementation of EnKF, two steps, namely forecast and analysis steps, are included (Evensen, 2003). First, the forecast state vector at the \( i + 1 \) moment is generated using the model operator and the analysis state vector at the \( i \) moment, which can be written as:

\[ X^{i+1}_f = M X^i \]  

in which \( X^{i+1}_f \) is the forecast state vector, and \( X^i \) is the analysis state vector.

When the observation data is available, the analysis state vector is updated using the analysis equation, which can be written as:
\[ X_{i+1}^j = X_{i+1}^{j+1} + K_{i+1} (Y_{i+1} + e_{i+1}^j - H_{i+1} X_{i+1}^{j+1}) \]  
where \( K_{i+1} \) is the Kalman gain, which is defined as:

\[ K_{i+1} = P_{i+1} H_{i+1}^T (H_{i+1} P_{i+1} H_{i+1}^T + O_{i+1})^{-1} \]

where \( P_{i+1} \) is the predictive error covariance matrix, which can be expressed as follows:

\[ P_{i+1} = \frac{1}{J-1} \sum_{j=1}^{J} (X_{i+1}^{j+1} - \bar{X}_{i+1}^{j+1})(X_{i+1}^{j+1} - \bar{X}_{i+1}^{j+1}) \]

in which \( \bar{X}_{i+1}^{j+1} \) is the mean of \( X_{i+1}^{j+1} \). The damping factor (Hendricks Franssen and Kinzelbach, 2008) was used to reduce the inbreeding problem, hence the Eq. (9) is revised as:

\[ X_{i+1}^j = X_{i+1}^{j+1} + \beta K_{i+1} (Y_{i+1} + e_{i+1}^j - H_{i+1} X_{i+1}^{j+1}) \]

where \( \beta \) is the damping factor, with values between 0 and 1. In this study, \( \beta \) is considered with a value of 0.1.

In this study, two assimilation strategies are considered. The main difference between the two strategies is the selection of the model operator and the observation operator. In strategy 1 (S1), the soil hydrodynamic model is used as the model operator. Because the observation data includes soil moisture or pressure head, the observation operator is a unit matrix \( I \). The state variables and model parameters are updated using the state augmentation technique. In strategy 2 (S2), the state vector consists of soil hydraulic parameters, and the model operator is a unit matrix \( I \). Since parameters are treated as state variables, S2 is called the parameter correction method. The soil hydrodynamic model provides a direct link between parameters and observation elements (soil moisture or pressure head), and hence the Richards equation is the nonlinear observation operator. In each assimilation strategy, two-parameter update methods are further analyzed. In method 1 (M1), parameters are updated simultaneously. In method 2 (M2), parameters
are updated separately, i.e., the partitioned update method (Xie and Zhang, 2013). Therefore, a total of four assimilation schemes, namely the simultaneous update state augmentation method (S1M1), the partitioned update state augmentation method (S1M2), the simultaneous update parameter correction method (S2M1), and the partitioned update parameter correction method (S2M2) are compared in this study.

3. Case study

3.1. Synthetic case

In the synthetic case, water infiltration from a single-ring infiltrometer into a layered soil was simulated. The soil profile consists of two layers: 40 cm thick A-horizon and an underlying B/C-horizon. The hydraulic parameters of two soil layers are shown in Table 1 (Císlérová, 1987; Hopmans and Stricker, 1989). Fig. 1 presents the axisymmetric computational domain. The computational domain was discretized into 684 finite elements. All sides of the computational domain are impermeable except for a small portion around the origin at the soil surface where a constant pressure head was imposed and the lower right corner where the groundwater level was kept constant. The initial pressure

| Table 6 |
| RMSE of the estimated parameters for four assimilation schemes. |

<table>
<thead>
<tr>
<th>Periodic variation</th>
<th>Linear variation</th>
<th>Abrupt change</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_s$ (cm min$^{-1}$)</td>
<td>$a$ (cm$^{-1}$)</td>
<td>$K_s$ (cm min$^{-1}$)</td>
</tr>
<tr>
<td>S1M1</td>
<td>0.0025</td>
<td>0.0007</td>
</tr>
<tr>
<td>S1M2</td>
<td>0.0026</td>
<td>0.0003</td>
</tr>
<tr>
<td>S2M1</td>
<td>0.0026</td>
<td>0.0004</td>
</tr>
<tr>
<td>S2M2</td>
<td>0.0026</td>
<td>0.0002</td>
</tr>
</tbody>
</table>

| Table 7 |
| Correlation coefficient of the estimated parameters for a single time-varying parameter. |

<table>
<thead>
<tr>
<th>Periodic variation</th>
<th>Linear variation</th>
<th>Abrupt change</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1M1</td>
<td>0.99</td>
<td>0.99</td>
</tr>
<tr>
<td>S1M2</td>
<td>0.61</td>
<td>0.54</td>
</tr>
<tr>
<td>S2M1</td>
<td>0.99</td>
<td>0.99</td>
</tr>
<tr>
<td>S2M2</td>
<td>0.45</td>
<td>0.34</td>
</tr>
</tbody>
</table>

Fig. 4. Absolute errors for simulated pressure head distributions (cm) for four assimilation schemes: (a) $K_s$ has a periodic variation, (b) $K_s$ has a linear variation, (c) $K_s$ has an abrupt change.
head profile and locations of observation points are shown in Fig. 1b. The ensemble size was set to 300, which has been tested to be large enough to meet the accuracy requirements, i.e., the relative errors of estimated parameters are less than 5%. Shi et al. (2015) reported that the type of observation data might affect assimilation results. To better test the ability of the assimilation methods to identify time-varying parameters, pressure heads were chosen as the observation data in this case. The total simulation time was 10 days, and pressure heads at observation points were recorded every 2 h. The measurements were obtained by adding an observation error to the pressure heads simulated using the true parameters. The standard deviation of the observation error is 0.01 m. The parameters to be estimated are $K_S$ and $\alpha$ of the first soil layer because they are the most variable parameters (Carsel and Parrish, 1988). Estimated parameters were log-transformed because their probability distributions are known to approximate lognormal distributions (Carsel and Parrish, 1988). The standard deviation of the initial parameter ensemble is 0.1 for both $\log_{10}(K_S)$ and $\log_{10}(\alpha)$.

To test the ability of assimilation methods on identifying the dynamics of parameters, multiple scenarios, in which parameters have different time variation trends, were designed. First, only a single time-varying parameter was considered, i.e., $K_S$ changed with time, and $\alpha$ was constant. Different variation trends of $K_S$ were developed, i.e., a periodic variation, a linear variation, and an abrupt change. Similar assumptions of parameter variations were also used by Deng et al. (2016) and Xiong et al. (2019). Second, to check the parameter correlation issue that may arise during the assimilation, both $K_S$ and $\alpha$ were considered to change with time. Two scenarios were designed in this case: (1) $K_S$ has a periodic variation, and $\alpha$ has an abrupt change. The results of four assimilation schemes were compared with each other.

### Table 8

<table>
<thead>
<tr>
<th>Scenario 1</th>
<th>Scenario 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1M1</td>
<td>0.99</td>
</tr>
<tr>
<td>S1M2</td>
<td>0.89</td>
</tr>
<tr>
<td>S2M1</td>
<td>0.99</td>
</tr>
<tr>
<td>S2M2</td>
<td>0.84</td>
</tr>
</tbody>
</table>

### Table 9

<table>
<thead>
<tr>
<th>Scenario 1</th>
<th>Scenario 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_S$ (cm min$^{-1}$)</td>
<td>$\alpha$ (cm$^{-1}$)</td>
</tr>
<tr>
<td>------------</td>
<td>------------</td>
</tr>
<tr>
<td>S1M1</td>
<td>0.0044</td>
</tr>
<tr>
<td>S1M2</td>
<td>0.0040</td>
</tr>
<tr>
<td>S2M1</td>
<td>0.0041</td>
</tr>
<tr>
<td>S2M2</td>
<td>0.0032</td>
</tr>
</tbody>
</table>

3.2. Real case

A field drip irrigation experiment with processing tomatoes was conducted at the upper reaches of the Yellow River basin, China (latitude 40°41’N, longitude 107°18’E, and 1041 m altitude). The soil profile 60 cm deep can be divided into three layers. The physical properties of the three soil layers are given in Table 2. The growth period started from 6/2/2015 and lasted till 9/1/2015, i.e., 104 days in total. According to
FAO-56 (Allen et al., 1998), the growth period of processing tomatoes can be divided into four growth stages (see Table 3). Meteorological data was measured by an automatic weather station (HOBO, Campbell Scientific Inc., USA). Daily reference evapotranspiration (ETo) was calculated using the modified Penman-Monteith equation (Allen et al., 1998). Soil water contents at two horizontal locations and three depths (Fig. 2) were monitored using HydraProbe sensors. The computational domain, boundary conditions, and the position of observation points are shown in Fig. 2. The computational domain was discretized into 2527 finite elements. A time-variable flux boundary condition, determined from irrigation rates, was specified on the BC boundary (Fig. 2). The drip flux during the growth period is given in Table 4. A no flux boundary condition was specified on the CD side because of a plastic mulch cover, and an atmospheric boundary condition was specified on the DE side. The lower boundary was treated as a free drainage boundary because the groundwater table was relatively deep. Due to symmetry of flow, a no flux boundary condition was specified on both vertical sides. Water uptake was simulated using the model of Feddes et al. (1978) with default values of parameters of the stress response function provided by HYDRUS-2D (Siminek et al., 2012). The initial water content was 0.4 cm$^{-3}$, 0.37 cm$^{-3}$, and 0.45 cm$^{-3}$ in depths of 0–20 cm, 20–40 cm, and 40–60 cm, respectively. An ensemble size of 300 and a 1-day interval were used in the assimilation. A value of 0.01 was used as the standard deviation for the soil water content observation error (Shi et al., 2015). According to Haverkamp et al. (1996), the parameters $\theta_S$, $K_S$, and $\alpha$ depend on the soil structure, and hence these three parameters of the soil top layer were estimated. Initial values of soil hydraulic parameters of the three soil layers (shown in Table 5) were obtained using the Levenberg-Marquardt optimization algorithm (Moré, 1978). The standard deviation of the initial parameter ensemble was 0.1 for log$_10(K_S)$ and log$_10(\alpha)$, and 0.02 for $\theta_S$. The parameter estimations and water content simulations obtained using the partitioned update parameter correction method are compared with those of the traditional state augmentation method.

### 3.3. Evaluation index

The root mean square error (RMSE) is used to evaluate parameter estimations for the synthetic case and simulated soil water contents for the real case. The absolute error (AE) is used to evaluate the simulated pressure head distribution.

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (S_i - O_i)^2}$$

$$AE = S_i - O_i$$

where $N$ is the total number of observations, $S_i$ and $O_i$ are the $i$th model-simulated and observed values, respectively.

The Pearson correlation coefficient ($R$) is used to analyze the linear relationship between estimated parameters.

$$R = \frac{\sum_{i=1}^{N} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{N} (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^{N} (y_i - \bar{y})^2}}$$

where $x$ and $y$ denote different model parameters; and $\bar{x}$ and $\bar{y}$ are the mean values of these parameters.

**Fig. 6.** Absolute errors of simulated pressure head distributions (cm) for Scenario 2.
4. Result and discussion

4.1. Single time-varying parameter

Fig. 3 presents the evolutions of the estimated parameters. When $K_S$ has a periodic variation, estimated $K_S$ values show significant time-lags compared with the true value variation. This is consistent with the results of Clark et al. (2008), Samuel et al. (2014), Deng et al. (2016), and Xiong et al. (2019). This is due to the defect in the EnKF method. The states and parameters are updated based on current observations and previous predictions, and hence there is a time lag between the assimilation value estimated using the EnKF method and the true value, especially when a peak value occurs (Clark et al. 2008). The estimated $K_S$ peak value is lower compared to its true value, especially for the simultaneous update method (M1). This may be attributed to the mutual influence between estimated parameters. As can be seen from Fig. 3(a), the parameter $\alpha$ estimated using the simultaneous update method (M1) has a large deviation from its true value, which in turn affects the estimation of $K_S$. The parameter $\alpha$ estimated using the partitioned update method (M2) can eventually converge to its true value.

When $K_S$ has a linear variation, values of $K_S$ estimated by the four assimilation schemes are lower than the true value. This can also be

Fig. 7. Parameter evolutions for different initial parameter values [(a) Equal to the true value, (b) Larger than the true value, (c) Less than the true value].

Table 10
RMSE of the estimated parameters for different initial parameter values.

<table>
<thead>
<tr>
<th>Larger</th>
<th>Equal</th>
<th>Less</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_S$ (cm min$^{-1}$)</td>
<td>$\sigma$ (cm$^{-1}$)</td>
<td>$K_S$ (cm min$^{-1}$)</td>
</tr>
<tr>
<td>S1M1</td>
<td>0.0044</td>
<td>0.0022</td>
</tr>
<tr>
<td>S1M2</td>
<td>0.004</td>
<td>0.0016</td>
</tr>
<tr>
<td>S2M1</td>
<td>0.0041</td>
<td>0.0023</td>
</tr>
<tr>
<td>S2M2</td>
<td>0.0032</td>
<td>0.0018</td>
</tr>
</tbody>
</table>
regarded as a time lag for the parameter estimation. Values of parameter $\alpha$ estimated using the simultaneous update method (M1) show large deviations from its true value. On the other hand, the parameter $\alpha$ estimated using the partitioned update method (M2) can converge to its true value.

When $K_S$ has an abrupt change, all four assimilation schemes could respond to the abrupt change of the parameter value immediately. However, multiple assimilation operations (about 50 assimilations in this case) are required for the parameter to converge to its true value. The parameter $\alpha$ was overestimated using the simultaneous update method (M1). The partitioned update method (M2) could obtain accurate $\alpha$ estimation.

Fig. 8. Absolute errors of simulated pressure head distributions (cm) for different initial parameter values [(a) Larger than the true value, (b) Equal to the true value, (c) Less than the true value).

Fig. 9. Parameter evolutions for different parameter update orders.
Table 6 gives the RMSE values for the estimated parameter for four assimilation schemes. It can be found that the partitioned update method (M2) obtains more accurate results except for the case of a periodically varying $K_S$. Low RMSE values for the case of a periodic varying $K_S$ may be attributed to the time lags of parameter estimation. Standard deviations of the parameters are similar for four assimilation schemes (see Fig. 3). Standard deviations have dropped to a very low level after 50 assimilations.

As can be seen from Fig. 3, there is an obvious parameter correlation issue, i.e., the evolutions of $\alpha$ display similar trends as $K_S$ when the parameters are updated simultaneously, which results in low estimation accuracy of $\alpha$. Compared with the simultaneous update method, parameter correlation coefficients decrease significantly for the partitioned update method, especially when the parameter correction method is used (see Table 7). This indicates that the partitioned update method can effectively resolve parameter correlation issues, thereby improving the accuracy of parameter estimations.

Simulated pressure head error distributions for four assimilation schemes are shown in Fig. 4. Simulation errors in the 30–70 cm soil depth are large, which is caused by the parameter estimation error. Except for a periodically varying $K_S$, simulated pressure head distributions using parameters obtained by the partitioned update method are more accurate than those using parameters obtained by the simultaneous update method because of better parameter estimations. This is consistent with the results of Xie and Zhang (2013). For the case with a periodically varying $K_S$, due to the time lags of parameter estimations, the accuracy of simulated pressure head distributions is similar for four assimilation schemes.

### 4.2. Multiple time-varying parameters

Fig. 5 presents the parameter evolutions for different parameter variation scenarios, i.e., for Scenario 1 with a periodic variation of $K_S$ and a linear trend in $\alpha$, and Scenario 2 with a periodic variation of $K_S$ and an abrupt change in $\alpha$. It can be found that there are obvious parameter correlations in the parameter estimations using the simultaneous update method. The estimated $K_S$ has the same increasing trend as the $\alpha$ parameter in Scenario 1. The evolution of $K_S$ showed a significant inflection point with an abrupt change of $\alpha$ in Scenario 2. The correlation coefficients of the estimated parameters are given in Table 8. The $R$ values for the partitioned update method are smaller, resulting in a higher accuracy of parameter estimation (see Table 9). Deng et al. (2016) and Xiong et al. (2019) successfully estimated time-varying parameters of a two-parameter water balance model (Xiong and Guo, 1999) using the simultaneous update state augmentation method. However, four assimilation schemes cannot obtain the ideal estimation of time-varying soil hydraulic parameters in our study. This may be attributed to the fact that the Richards equation has stronger nonlinear properties compared to a two-parameter water balance model. Since simulated pressure head error distributions for Scenarios 1 and 2 are similar, Fig. 6 only presents the results for Scenario 2. The accuracy of pressure head simulations using parameters obtained by the partitioned

<table>
<thead>
<tr>
<th></th>
<th>$K_S$ (cm min$^{-1}$)</th>
<th>$\alpha$ (cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1 – $K_S \alpha$</td>
<td>0.004</td>
<td>0.0016</td>
</tr>
<tr>
<td>S1 – $\alpha K_S$</td>
<td>0.0028</td>
<td>0.0018</td>
</tr>
<tr>
<td>S2 – $K_S \alpha$</td>
<td>0.0032</td>
<td>0.0018</td>
</tr>
<tr>
<td>S2 – $\alpha K_S$</td>
<td>0.0032</td>
<td>0.0019</td>
</tr>
</tbody>
</table>

Fig. 10. Absolute errors of simulated pressure head distributions (cm) for different parameter updating orders.
update parameter correction method is the highest among the four schemes because of good parameter estimations.

4.3. Effect of the initial parameter value

Since there is uncertainty in the selection of initial values of estimated parameters in practical applications, the effects of the initial parameter value on assimilation are analyzed next. Fig. 7 presents the parameter evolutions for different initial parameter values. It can be found that the time lags of the estimated parameter cannot be avoided regardless of the initial parameter value. When the parameters’ initial values are greater than their true values, the trends in parameter estimation are similar to when the initial parameter values are equal to their true values. However, when the parameters’ initial values are smaller than their true values, the parameter estimation accuracy is significantly reduced (Table 10), which leads to inaccurate simulations of pressure head distributions (see Fig. 8). This can be attributed to the fact that smaller saturated hydraulic conductivity results in slower reactions to forcing. If soil water dynamics is slow, parameters cannot be estimated well. And if the van Genuchten $\alpha$ is low, the pressure entry head is high, and the soil is wet, and forcing will not have a strong effect. This makes parameter estimation more difficult. The results indicate that when the initial value of the optimized parameter deviates from the true value to a certain extent, even the partitioned update method cannot obtain accurate parameter estimations and soil moisture simulations.

4.4. Effect of the parameter update order

For the partitioned update method, the parameter update order may influence the parameter estimations (Xie and Zhang, 2013). Therefore, the effect of the parameter update order is further investigated. Fig. 9 presents the parameter evolutions for different parameter update orders. For the partitioned update state augmentation method, updating $K_S$ first can result in better estimation accuracy of $\alpha$. Conversely, updating $\alpha$ first can improve the estimation accuracy of $K_S$ (Table 11). This may be because the accuracy of simulated pressure heads is improved when the first parameter is updated, which is beneficial for updating the second parameter. On the other hand, the parameter update order has only a small influence on the estimations for the partitioned update parameter correction method (Table 11), because the parameters and state variables are not updated simultaneously in the parameter correction method. Simulated pressure head error distributions are shown in Fig. 10. For the partitioned update state augmentation method, updating $\alpha$ first can improve the simulation accuracy, which indicates that in this example, the simulation is more sensitive to the parameter $K_S$. Hence the parameter update order needs to be carefully selected when the partitioned update state augmentation method is used. Xie and Zhang (2013) recommended that the parameter updating order should be performed in the order of increasing sensitivity. In contrast, the partitioned update parameter correction method can obtain good results of parameter estimations and simulations regardless of the parameter update order.

4.5. Application to the drip irrigation experiment

Fig. 11 presents the parameter evolutions for the drip irrigation experiment when the partitioned update parameter correction method and the traditional state augmentation method are used. For comparison, constant parameter values obtained using the Marquardt-Levenberg optimization method are also shown. Fig. 11 shows that $\theta_S$ did not change much during the growth period, and estimated $\theta_S$ values using the partitioned update parameter correction method were similar to those obtained using the traditional state augmentation method. The parameters estimated using the traditional state augmentation method showed larger fluctuations. The parameter values changed significantly after each rainfall or irrigation. This is because the parameters and soil water contents are updated simultaneously in the state augmentation technique. When the soil water content changed dramatically because of rainfall or irrigation, the model parameters also changed significantly. The parameters estimated using
The parameter values showed significant trend changes on days 5, 23, 27, and 68. The values of α decreased after days 5, 23, and 68, which may be attributed to soil compaction due to rainfall or irrigation. The parameter variations were caused by the soil structure change rather than the assimilation errors in the previous simulations. In contrast, the parameters estimated using the traditional state augmentation method deviated from their true values, which could be attributed to unstable assimilation resulting from an increasing degree of freedom in the system (Moradkhani et al., 2005).

Due to a large number of state variables in the simulations of multi-dimensional soil water flow, the size of the matrix to be updated in the traditional state augmentation method is larger than in the partitioned update parameter correction method, leading to much more computational time. The state augmentation method is prone to an inconsistency problem during assimilations, resulting in non-convergence of the iterative solution of the Richards equation, which makes the assimilation unstable. This is because the unsaturated water flow is a highly nonlinear problem, and the assimilation of state variables and parameters using the linear equation may not follow the nonlinearity of the Richards equation (Song et al., 2014). Since only parameters are assimilated in the partitioned update parameter correction method, the inconsistency problem may be avoided. Therefore, in multi-dimensional unsaturated water flow problems, using the partitioned update parameter correction method can improve the calculation efficiency and the assimilation stability while obtaining more accurate parameter estimations and soil moisture predictions.

It should be noted that the sequential data assimilation requires consecutive data to achieve statistical convergence of parameter estimation. If the observation data is not enough, the parameter may not converge to its true value, especially for parameters with specific (such as linear) trend. Hence, a small assimilation time interval or a long time-series of data are required to improve the convergence of parameter estimates for short-period simulation. For example, tillage practice may result in the temporal variation of soil parameters. In this study, tillage practice’s temporal variation of soil parameters was not considered since the tillage occurred before crop transplanting, and the soil...
structure had stabilized when crop growth began. However, the proposed assimilation method can also be applied to soil disturbed by tillage practice if sufficient observation data can be obtained.

In the real test case, on the one hand, the change of boundary conditions, e.g., time-varying irrigation flux and evapotranspiration, and root growth might cause the change of soil structures, leading to time-varying parameters. Compared with the traditional methods, the partitioned update parameter correction method can improve soil moisture predictions. On the other hand, soils are heterogeneous, which cannot be well captured by available models. This will result in the predictions deviating from the observations. The partitioned update parameter correction method provides an efficient tool for assimilating multi-dimensional soil water flow by considering the time-varying parameters representing the influence of all relevant factors, e.g., soil heterogeneity, change of boundary conditions, root growth and model errors, etc. However, it should be mentioned that the temporal change of parameters is inherent in the assimilation method and that there can be other reasons why parameters change during the updates. Most of these reasons are related to experimental and modeling errors. For example, the measurement errors, simplifications of initial and boundary conditions, inadequacy of governing transport equations to describe observed processes fully (e.g., the presence of preferential flow during rainfalls), etc., can also result in assimilation methods predicting temporal variations of optimized parameters.

5. Summary and conclusions

In this study, we explored the potential of the assimilation method to estimate time-varying soil hydraulic parameters. Four assimilation schemes were compared, including the simultaneous update state augmentation method, the partitioned update state augmentation method, the simultaneous update parameter correction method, and the partitioned update parameter correction method. The four assimilation schemes’ performance on parameter estimation and soil moisture simulations were first tested using the synthetic case. The influence of the initial parameter value and the parameter update order on assimilation was also analyzed. The partitioned update parameter correction method was then applied to a real case involving a field drip irrigation experiment. The results showed that when the parameter had a periodical or a linear variation, there were time lags between the assimilation value and the true value. The assimilation method could respond to an abrupt change of the parameter value immediately. There were obvious parameter correlation issues when the simultaneous update method was used. The partitioned update method could effectively resolve the parameter correlation issue, thereby improving the accuracy of parameter estimations and pressure head simulations. However, when the initial values of the parameters deviated from their true values to a certain extent, the partitioned update method could not obtain accurate parameter estimations. The partitioned update parameter correction method was not sensitive to the parameter update order. Since only parameters are updated in the assimilations, the inconsistency of the assimilation could be avoided. Compared with the traditional state augmentation method, the partitioned update parameter correction method has high computational efficiency and assimilation stability, it provides an efficient tool for the assimilation of multi-dimensional unsaturated water flow problems by considering the time-varying parameters.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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