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Dual state-parameter estimation of root zone soil moisture by optimal parameter estimation and extended Kalman filter data assimilation

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ABSTRACT

With well-determined hydraulic parameters in a hydrologic model, a traditional data assimilation method (such as the Kalman filter and its extensions) can be used to retrieve root zone soil moisture under uncertain initial state variables (e.g., initial soil moisture content) and good simulated results can be achieved. However, when the key soil hydraulic parameters are incorrect, the error is non-Gaussian, as the Kalman filter will produce a persistent bias in its predictions. In this paper, we propose a method coupling optimal parameters and extended Kalman filter data assimilation (OP-EKF) by combining optimal parameter estimation, the extended Kalman filter (EKF) assimilation method, a particle swarm optimization (PSO) algorithm, and Richards' equation. We examine the accuracy of estimating root zone soil moisture through the optimal parameters and extended Kalman filter data assimilation method by using observed in situ data at the Meiling experimental station, China. Results indicate that merely using EKF for assimilating surface soil moisture content to obtain soil moisture content in the root zone will produce a persistent bias between simulated and observed values. Using the OP-EKF assimilation method, estimates were clearly improved. If the soil profile is heterogeneous, soil moisture retrieval is accurate in the 0–50 cm soil profile and is inaccurate at 100 cm depth. Results indicate that the method is useful for retrieving root zone soil moisture over large areas and long timescales even when available soil moisture data are limited to the surface layer, and soil moisture content are uncertain and soil hydraulic parameters are incorrect.

1. Introduction

Soil moisture content in the root zone is an important state variable in many aspects of studies in hydrology, meteorology and agriculture. In hydrological research, soil water content plays a key role in the partitioning of rainfall into infiltration and runoff ([54,30,56]). In meteorological research, soil water content has a crucial effect on the partitioning of available energy at the earth's surface into sensible and latent heat exchange with the atmosphere [29]. In agriculture, soil moisture is essential for proper water resource management, irrigation scheduling, crop production, and chemical monitoring [18,19,31]. Obtaining accurate soil moisture data sets at large scales over a long period is not an easy task [40]. Measurements of in situ soil moisture are usually expensive and time-consuming. Moreover, there are no large-scale soil moisture observational networks available for measuring soil moisture at high temporal frequency at multiple soil depths. In recent years, several research efforts have focused on the development of remote-sensing techniques to characterize the spatial and temporal variability of soil moisture over large regions [4,24,23,33]. Many of these studies have successfully demonstrated that the use of passive microwave remote sensors can obtain soil moisture content [2,16,17]. Though much progress has been made, these developments have been limited in that they characterize soil moisture in a rather shallow layer, variously estimated between 2 and 20 cm deep, but mostly 5 cm deep [26].

To estimate soil moisture profile (or root zone soil moisture) with the help of surface soil moisture observations is an important research problem. Jackson [25] described four basic approaches using surface soil moisture data to estimate soil moisture throughout a soil profile. However, current research emphasis has focused on the assimilation of remotely sensed surface soil moisture data into different types of hydrological models. Analysis using data assimilation provides time-dependent spatially distributed soil moisture content estimates that can be updated whenever new data become available. There are many alternative assimilation methods, such as direct insertion, Kalman filters [52,42], and

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H-infinity filters [53]. The application of these assimilation methods to accurately estimate soil moisture in a profile is a relatively new and challenging area of investigation.

In combining assimilation methods with hydrological models and climatic models to retrieve root zone soil moisture in a soil profile, soil hydraulic parameters are essential inputs to most hydrological and climatic models [34,35]. However, these essential soil hydraulic parameters are not always available for practical applications. On the other hand, during the past two decades, much effort has been directed toward the estimation of hydrologic model parameters (calibration) to improve the forecast accuracy. Only a few studies have been performed based on dual state-parameter estimation of hydrological models (or flood forecast models), [39,49,8,14]. In the study of soil moisture forecasting, most data assimilation methods examine only how to update the state variables (soil moisture content), and studies exploring how to update soil hydraulic parameters are neglected. When the key parameters are incorrect, the assimilation results may be affected and the assimilation process may fail. For example, a main assumption of the Kalman filter is that the model errors are zero mean and uncorrelated in time. This assumption is commonly violated in hydrological applications, and the model can be biased. Especially when a key parameter (such as the saturated hydraulic conductivity, K_s) is largely overestimated, the Kalman filter-based assimilation approach is not sufficient for removing persistent bias in the soil water balance [37]. Indeed, the filter assumption (mean zero of the model error) is violated. Montaldo et al. [38] examined the effect of uncertain saturated hydraulic conductivity (K_s) on assimilation performance. They concluded that the erroneous estimation of K_s may bring about a long-term error for simulated results. This error is not removed by using the assimilation method. Das and Mohanty [9] concluded that uncertainties introduced by soil hydraulic properties caused suboptimal performance of a retrieval model using the ensemble Kalman filter technique. Moradkhani et al. [39] showed that good estimates of the parameters and state variables are needed to enable the model to generate accurate forecasts. In their paper, they studied a dual state-parameter estimation approach based on the ensemble Kalman filter [14] for sequential estimation of both parameters and state variables of a hydrologic model. On the other hand, in Chen and Zhang's [6] paper, the ensemble Kalman filter approach is used for continuous updating model parameters and motel state variable with large ensembles sizes. In van Der Merwa and Wan's [49], the square root unsigned Kalman filter (SR-UKF) is used for continuous updating model parameters and model state variables. These studies, however, do not apply for soil moisture forecasting and research related to simultaneously estimating soil parameters and state variables at the same time is sparse.

In this paper, we develop a method of coupling of optimal parameters and extended Kalman filter data assimilation (OP-EKF) by combining an inverse modeling-based state-parameter assimilation strategy and a state variable soil moisture assimilation method. This is unlike previous near-surface data assimilation procedures where root zone soil moisture is being retrieved [12,15,52,20,11,10]. The methodology has two steps which are necessary for capturing the persistent model bias: (1) it dynamically adjusts (i.e., calibrates) the needed soil hydraulic parameters at the root zone at a coarse time scale, by deriving the needed soil hydraulic parameters by combining a PSO algorithm [28,7] and a hydrological model, then inserting the obtained soil hydraulic parameters into the hydrological model; and (2) it simulates the root zone soil moisture content by assimilating surface soil moisture data using the EKF method at the observation time scale. In this study, we verify the effectiveness of this method by using field data on soil moisture collected from the Meiling experimental station, China. Our study was designed to test the coupling optimal parameters and extended Kalman filter data assimilation method under "real-world" conditions and to evaluate the value of using actual field data. Our work also explores the possibility of retrieving a root zone soil moisture profile under some unknown soil hydraulic parameters and uncertain initial soil moisture content.

2. Methodology

2.1. Study area description

Field experiments were conducted at the Meiling experimental watershed (31°0′N, 119°1′E), Jiangsu Province, China. The watershed area is about 0.7 km^2, located about 9 km west of Tai Lake. The average annual rainfall over the last 30 years is about 1150 mm, and average annual temperature is about 15.5 °C. Long-term soil moisture observation equipment was installed on a hillside in the upper part of the watershed. The vegetation on the hillside is chestnut woodland and canopy cover is high. The root depth is about 100 cm. There are forbs on the ground in summer. The soil physical particle size values at all depths were measured by the laser diffraction method (Table 1).

In the experimental area, there are four frequency domain reflector (FDR) soil moisture sensors at 5, 30, 50 and 100 cm depths. Voltage readings (mV) were recorded every hour. Volumetric soil moisture content was computed according to the "voltage-volume moisture content curve", which is determined in accordance with measured samples. Data measurements were taken from November 16, 2006 to November 7, 2007. The simulation performed begins at July 1, 2007 (DOY 182), and ends at August 31, 2007 (DOY 243). In the simulation cycle, there were four days (DOY 218–221) in which the equipment was malfunctioning.

In addition to the measurements of soil moisture, some meteorological observations were recorded, including: wind direction, wind speed, E601-water surface evaporation, temperature, humidity, vapor pressure deficit, saturated vapor pressure deficit, relative humidity, solar radiation, precipitation, and soil temperature at different depths.

2.2. Governing equation

The system equations in the assimilation scheme are based on the one-dimensional (1-D) Richards' equation that describes moisture fluxes in the unsaturated zone of a homogeneous and isotropic soil. The 1-D mixed Richards' equation can be written as:

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

where θ is the soil water content (cm^3 cm^{-3}), z is the soil depth (cm), h is the soil water pressure head (cm), K is the unsaturated hydraulic conductivity (cm d^{-1}), and $S(t,z,h)$ is the root water uptake (cm d^{-1}). The van Genuchten [47] relationships are used to express the dependence between K and the state variable (either pressure head h or moisture content θ) of interest:

Table 1
The average soil physical properties with depth in the experimental plot.

Depth (cm)	% Sand	% Silt	% Clay	Bulk density (g cm^{-3})
0–5	13.7	70.6	15.7	1.35
5–18	13.7	70.7	15.6	1.39
18–54	14.9	67.7	17.4	1.26
54–74	17.5	74.9	7.6	1.41
74–120	18.6	75.0	6.4	1.29

Clay, silt and sand were defined as particles <0.002, 0.002–0.05 and 0.05–2.0 mm in diameter, respectively.