Advances in Water Resources 91 (2016) 104–116

Contents lists available at ScienceDirect

Advances in Water Resources

journal homepage: www.elsevier.com/locate/advwatres

Estimating soil moisture and soil thermal and hydraulic properties by assimilating soil temperatures using a particle batch smoother

Jianzhi Dong[a,*], Susan C. Steele-Dunne[a], Tyson E. Ochsner[b], Nick van de Giesen[a]

[a] Water Resources Section, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Delft, Netherlands
[b] Department of Plant and Soil Sciences, Oklahoma State University, Stillwater, Oklahoma, USA

ARTICLE INFO

Article history:
Received 8 September 2015
Revised 16 March 2016
Accepted 17 March 2016
Available online 19 March 2016

Keywords:
Soil temperature
Soil moisture
Soil properties
Data assimilation
Hydrus 1-D

ABSTRACT

This study investigates the potential of estimating the soil moisture profile and the soil thermal and hydraulic properties by assimilating soil temperature at shallow depths using a particle batch smoother (PBS) using synthetic tests. Soil hydraulic properties influence the redistribution of soil moisture within the soil profile. Soil moisture, in turn, influences the soil thermal properties and surface energy balance through evaporation, and hence the soil heat transfer. Synthetic experiments were used to test the hypothesis that assimilating soil temperature observations could lead to improved estimates of soil hydraulic properties. We also compared different data assimilation strategies to investigate the added value of jointly estimating soil thermal and hydraulic properties in soil moisture profile estimation. Results show that both soil thermal and hydraulic properties can be estimated using shallow soil temperatures. Jointly updating soil hydraulic properties and soil states yields robust and accurate soil moisture estimates. Further improvement is observed when soil thermal properties were also estimated together with the soil hydraulic properties and soil states. Finally, we show that the inclusion of a tuning factor to prevent rapid fluctuations of parameter estimation, yields improved soil moisture, temperature, and thermal and hydraulic properties.

1. Introduction

Recent research has shown the potential of using Distributed Temperature Sensing (DTS) to provide insights into soil moisture spatial variability [1–4]. DTS uses fiber optic cables to measure soil temperatures with high resolutions (temporal resolution less than 1 minute, and spatial resolution less than 1 m) up to kilometers [5]. Soil temperature change due to the thermal responses, either to electrically-generated heat pulses (Active DTS) or net solar radiation (Passive DTS), can be measured using DTS. This temperature change can be linked to soil moisture using empirically calibrated or physically based functions (e.g. soil thermal conductivity and diffusivity curve) [1–4]. Active DTS methods are relatively accurate, particularly when soil moisture is low [2–4]. However, the electrical energy requirement may be a logistical obstacle for some field applications. Passive DTS, which requires no artificial input energy for heat pulses, can be used to estimate the soil thermal diffusivity using the evolution of soil temperature within a 24 hour window [1]. The estimated soil thermal diffusivity can be used to interpret soil moisture dynamics. However, passive DTS may provide physically unreasonable estimates when solar radiation is low. In addition, soil thermal diffusivity is not a monotonic function of soil moisture, which complicates the inference of soil moisture. Finally, if the soil spatial variability is high, it may require intensive calibrations of the soil thermal diffusivity–moisture relationship.

Recent research demonstrated that soil moisture can be estimated by assimilating DTS measured soil temperatures into a fully coupled soil, water and vapor movement model (forward model) [6]. In data assimilation, the forward model provides a prior probability distribution of the soil states (i.e. soil moisture and temperature), and this prior will be updated (posterior) using the temperature observations. Data assimilation methods may be particularly suitable for DTS applications to account for spatial variability of soil properties. The soil temperature heating/cooling rate is mainly determined by the energy used for evaporation, which is essentially controlled by soil moisture. In addition, soil moisture affects the soil thermal properties, and hence the vertical propagation of soil heat. Soil temperature evolution within a certain window length may contain more information than instantaneous measurements. Consequently, a Particle Batch Smoother (PBS) was proposed to update soil moisture using

* Corresponding author. Tel.: +310619280101
E-mail address: jianzhi.dong@tudelft.nl (J. Dong).

http://dx.doi.org/10.1016/j.advwatres.2016.03.008
0309-1708/

the evolution of soil temperature within a certain window length [7]. The concept was tested using real world observations, which showed that soil moisture estimates at depth can be significantly improved by assimilating soil temperature at shallow depths.

Errors in soil thermal and hydraulic properties can lead to biased estimates of soil temperature and moisture states [8,9]. In data assimilation, a biased prior guess of soil thermal and hydraulic properties may also lead to inconsistency between the model states and parameters. While soil properties can be measured experimentally at the point scale, it is laborious and time consuming [10]. Thus, it might be infeasible for DTS applications if soil properties vary significantly in space. Furthermore, requiring intensive field measurements will also render the data assimilation methods less useful. Soil hydraulic and thermal properties can be modeled and approximated from easily measurable soil properties, e.g. soil texture and bulk density (e.g. [11–14]). However, calibrations using field measurements are usually required [15]. Alternatively, model parameters can be estimated jointly with model states (e.g. [16,17]). The state vector is augmented with the model parameters, and jointly updated by observations. Hence, the model states and parameters are more consistent. Synthetic studies showed that soil hydraulic properties can be estimated if surface soil moisture is assimilated [8,18,19]. The estimated model states, using dual state parameter estimation, are also generally better than those estimated by updating the states alone.

Previous studies have already demonstrated that soil thermal properties can be estimated using soil temperatures [1,20]. The hypothesis of this study is that soil hydraulic properties can also be inferred from soil temperature dynamics. A previous study has shown that the Particle Filter (PF) is usually superior to the Kalman filter in parameter estimation [21]. Previous work has shown that the PBS is superior to the PF because a series of soil temperature observations within the batch window contains more information than instantaneous measurements [7]. The hypothesis here is that because the parameters are time-invariant, the smoother (PBS) should be well-suited to estimate soil thermal and hydraulic properties.

First, Monte Carlo simulations will be used to illustrate the relationship between soil hydraulic properties, soil moisture, soil thermal properties and soil temperature. Then, a sensitivity study will be performed to identify the soil hydraulic parameters that have the most impact on soil temperature. The PBS will then be used for joint state-parameter estimation to estimate the soil temperature and moisture as well as the soil thermal and hydraulic properties. State-only (soil moisture and temperature) estimation will be compared to joint assimilation where soil thermal and/or hydraulic properties are also estimated. In addition to the quality of the parameter , we will also consider the benefit of parameter estimation on the soil and temperature state estimates. Finally, we will demonstrate that it is essential to use a tuning factor in the joint assimilation case to provide robust estimated model parameters and states.

Since the main scope of this study is to evaluate the performance of the PBS in joint state-parameter estimation, this study is limited to synthetic tests. Because the truth is perfectly known and the sources of uncertainty are also known by design, the performance of the PBS can be explicitly evaluated.

2. Method and materials

2.1. Hydrus-1D model

In this study, the vertical soil water, heat and vapor transport processes in the unsaturated zone are simulated using the Hydrus-1D model [22]. The governing equation for one-dimensional liquid and vapor flow is expressed as

Table 1
The primary model parameters and the function in the forward model.

Parameter	Notation	Type
θ_r	Residual water content	Hydraulic property
θ_s	Saturated water content	Hydraulic property
α	Air entry value	Hydraulic property
n	Shape parameter	Hydraulic property
K_s	Saturated soil water conductivity	Hydraulic property
ρ_b	Soil bulk density	Thermal property
Sand	Sand content	Thermal property
Clay	Sand content	Thermal property

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K_{Th}\frac{\partial h}{\partial z} + K_{Lh} + K_{TT}\frac{\partial T}{\partial z}\right] - S \tag{1}$$

where θ is the soil water content (m^3m^{-3}) at time t (s), and z is the vertical coordinate (positive upward) (m). K_{Th} and K_{TT} are the isothemal and thermal total hydraulic conductivities, respectively, and K_{Lh} is the isothermal unsaturated hydraulic conductivity. S is a sink term ($m^3m^{-3}s^{-1}$). K_{Lh} and the soil retention curve are determined using van Genuchten's model [23]:

$$K_{Lh} = K_s S_e^l \left[1 - (1 - S_e^{\frac{1}{m}})^m\right]^2 \tag{2}$$

$$\theta(h) = \begin{cases} \theta_r + \dfrac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \tag{3}$$

where K_s is the saturated hydraulic conductivity (ms^{-1}), S_e is the effective saturation, l, m, n and α are empirical shape parameters and θ_r and θ_s are the residual and saturated soil water contents (m^3m^{-3}), respectively.

The governing equation for soil heat transport is

$$\frac{\partial C_p T}{\partial t} + L_0\frac{\partial \theta_v}{\partial t} = \frac{\partial}{\partial z}\left[\lambda(\theta)\frac{\partial T}{\partial z}\right] - C_w\frac{\partial q_L T}{\partial z} - L_0\frac{\partial q_v}{\partial z} - C_v\frac{\partial q_v T}{\partial z} - C_w S T \tag{4}$$

where T is the soil temperature (K), C_w, C_v and C_p are the volumetric heat capacities of water, vapor and moist soil ($Jm^{-3}K^{-1}$), respectively,θ_v is the water content of water vapor (m^3/m^3), L_0 is the volumetric latent heat of vaporization of liquid water (Jm^{-3}), q_L and q_v are the flux densities of liquid water and vapor (ms^{-1}), respectively, and $\lambda(\theta)$ is the apparent soil thermal conductivity ($Wm^{-1}K^{-1}$). $\lambda(\theta)$ is estimated from

$$\lambda(\theta) = \lambda_0(\theta) + \beta_T C_w |q_L| \tag{5}$$

where β_T is the thermal dispersivity (m), and thermal conductivity λ_0 can be estimated in Hydrus-1D using either the Campbell model [12] or Chung and Horton model [24]. In this study, the Campbell model was used, because it can provide estimated soil thermal conductivity curve for any given soil texture, which is more preferable for synthetic tests [6]. A list of the primary model parameters are shown in Table 1.

For soil water movement, the upper boundary condition is "Atmospheric boundary condition with surface runoff." This means that the soil surface water fluxes were calculated based on the estimated precipitation and the vapor flux for a given meteorological forcing condition [22]. The lower boundary condition in the soil water transport model is "free drainage"

$$q_n = -K_{Lh}(h) \tag{6}$$

where q_n is the discharge rate, and $K_{Lh}(h)$ is the hydraulic conductivity corresponding to a pressure head of h. Soil heat fluxes