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Estimation of root zone soil moisture and surface fluxes partitioning using near surface soil moisture measurements

Jikang Li, Shafiqul Islam*

Cincinnati Earth System Science Program, Department of Civil and Environmental Engineering, University of Cincinnati, P.O. Box 210071, Cincinnati, OH 45221-0071, USA

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Abstract

We examine the feasibility of retrieving root zone soil moisture and partitioning of surface fluxes through a model inversion technique using surface measurements. Using a four-layer land surface model and observed datasets from Field Experiment (FIFE) 1987, we show that the sensitivities of surface soil moisture to deeper layer soil moisture are different to those of surface fluxes. Consequently, if one chooses the initial soil moisture profile that optimizes surface soil moisture, in a root mean square error sense, it may not lead to optimal estimation of surface fluxes. We also show that the accuracy of soil moisture profile retrieval from surface measurements depends strongly on the initial surface soil moisture conditions. For wetter surface conditions, an initialization based on remotely sensed surface soil moisture appears to be adequate for the retrieval of the soil moisture profile. For drier surface conditions, however, a decoupling of surface and deeper layer soil moisture might be triggered and an initialization based on surface soil moisture would lead to larger error. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

The soil moisture conditions both at the surface and at deeper layers control many near surface processes including partitioning of surface fluxes, ecosystem dynamics, and biogeochemical cycles. Intermittence in storm and interstorm dynamics, and heterogeneity in soil texture, vegetation, land use, and topography contribute to significant space–time fluctuations in soil moisture. Estimation of soil moisture states is an important issue for the initialization of current generation of land–atmosphere models. Currently, remote sensing techniques provide the most feasible capability to monitor soil moisture over a range of space and time scales (Schmugge et al., 1980; Jackson and Schmugge, 1989; Islam and Engman, 1996; Engman, 1997). Microwave techniques are widely used to quantitatively monitor soil moisture for a variety of topographic and vegetation conditions. Microwave measurements of soil moisture are, however, limited to the top few (less than 10) centimeters of the soil column.

Many land–atmosphere interaction processes depend on the profiles of the soil moisture and temperature to depths considerably larger than a few centimeters. Consequently, this shallow moisture sensing depth imposes a serious limitation on the use of passive microwave measurements of soil moisture

* Corresponding author. Tel.: +1-513-556-1026; fax: +1-513-556-2599.

E-mail address: shafiqul.islam@uc.edu (S. Islam).

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for land–atmosphere interaction studies. Over the last two decades, several promising approaches for the estimation of soil moisture profile have been proposed (Jackson, 1980; Camillo and Schmugge, 1983; Arya et al., 1983; Bruckler and Witono, 1989; Entekhabi et al., 1994). These approaches range from linear regression to knowledge based techniques that use prior information of hydrology and depth profile to inversion techniques that use combination of remotely sensed data and water balance models. Kostov and Jackson (1993) provided an excellent review of soil moisture profile estimation methods using remotely sensed surface moisture measurements. They concluded that proper integration and sequential assimilation of remote sensing of soil moisture and physical modeling appeared to be the most promising approach to solve the problem of profile soil moisture estimation. Attempts were also made to retrieve deeper layer soil moisture from near surface atmospheric variables (e.g. air temperature, humidity) by inverting a land surface model (Bouttier et al., 1993). This method assumes a close relationship between near surface atmospheric variables and soil moisture. Such an assumption is difficult to validate because the relationship is indirect and is confounded by other land surface and atmospheric effects (e.g. advection, topography, vegetation).

An alternative is to use remotely sensed surface variables (e.g. surface temperature) to retrieve the soil moisture profile through a model inversion. Recently, Calvet et al. (1998) used this methodology and suggested that knowing the atmospheric forcing and four or five estimations of the surface soil moisture over several days are adequate to retrieve the total soil water content by inverting a two-layer land surface model. They have argued that there is a strong relationship between the deeper layer soil moisture and surface soil moisture and hence, it is possible to infer soil moisture profile by optimizing the error in predicting surface soil moisture as a function of deeper layer soil moisture. This is an interesting proposition, and it has the potential to utilize remotely sensed surface soil moisture and a land surface model to estimate the soil moisture profile.

Capehart and Carlson (1997), on the other hand, argue that surface soil moisture may not be useful in knowing the column-average soil water content because during the drying phase a sharp vertical soil water gradient develops and surface soil moisture gets decoupled from the deeper layer soil moisture. In addition, estimation of the soil moisture profile from the optimized model predicted surface soil moisture does not necessarily mean that it would lead to accurate partitioning of fluxes.

Results from Calvet et al. (1998) and Capehart and Carlson (1997) highlight some of the difficulties associated with the retrieval of deeper layer soil moisture from surface and atmospheric information. A necessary precondition for Calvet et al. (1998) methodology is the existence of strong correlation between deeper layer soil moisture and surface soil moisture. Results from Capehart and Carlson (1997) suggest that such a correlation, if it exists, would strongly depend on the state of the surface soil moisture. We must mention, however, that Calvet et al. (1998) considered a surface layer corresponding to 0–50 mm layer while Capehart and Carlson (1997) studied a much shallower layer for thermal infrared applications. Thus, the relationship between the nature of decoupling and the depth of the soil layer cannot be fully discerned from these studies. We also note that a decoupling between the surface and deeper layer soil moisture is likely to be enhanced for a bare soil surface while it would be weakened by the vegetation cover. Such a decoupling is also likely to be dependent on leaf area index (LAI); larger LAI tends to mute the decoupling much more efficiently than smaller LAI.

Another issue which was not fully explored in the above studies is the adequacy of partitioning of surface fluxes as a function of retrieved soil moisture profile. This issue is critical for the coupling of land surface models with atmospheric models as well as for the determination of the sensitivity of surface fluxes to deeper layer soil moisture initializations. In this study, we will attempt to address some of these issues by using observed data sets from the First International Satellite Land Surface Climatology Project (ISLSCP) FIFE and a four-layer land surface model. In particular, we will examine the

- correlation between deeper layer soil moisture and surface soil moisture for various stages of wetting and drying and
- effects of deeper layer soil moisture initialization,

based on near surface soil moisture, on surface fluxes partitioning.

2. A brief description of the land surface model and data

2.1. Description of the land surface model

Manabe (1969) was perhaps the first to introduce the concept of interactive soil moisture in global climate models (GCMs) and has shown that interactive soil moisture has a significant influence on the temporal and spatial persistence of atmospheric processes. Since then, several studies have examined the role of interactive soil moisture at various temporal and spatial scales. Two general approaches are usually employed to represent temporal change of soil moisture at the land surface. The first approach does not use any prognostic equations for soil moisture dynamics but uses empirical relationships to calculate soil flux near the surface (Pielke, 1984; Deardorff, 1978). Because of their relative simplicity, variants of this approach are widely used in operational weather forecast and climate models. The second approach, on the other hand, uses a multilayer soil moisture with explicit prognostic equations for heat and moisture transport in the soil. Consequently, the second approach is more responsive to short term changes in surface and atmospheric conditions. This approach, however, requires additional soil related parameters and computational resources. As a result, use of this class of models has been largely confined within the research community models (McCumber and Pielke, 1981; Noilhan and Planton, 1989). Recently, Viterbo and Beljaars (1995) incorporated a four-layer detailed land surface scheme in the European Center for Medium range Weather Forecast (ECMWF) model. They have shown that this representation of soil moisture dynamics captures a wide range of time scales, from diurnal to seasonal to interannual scales, and improves the model performance significantly.

We will use a land surface model, developed based on the work of Viterbo and Beljaars (1995), in this study. This land surface model is designed to compute the different components of the surface energy and moisture budget and has four prognostic layers to calculate soil temperature and soil moisture. It can capture land surface dynamics from the diurnal cycle to seasonal time scales. The model of Viterbo and Beljaars (1995) has been tested extensively with the ECMWF model and several observational data sets, and found to capture the physical processes and time scales very well. Its surface parameterizations are derived from Deardorff (1977, 1998), Abramopoulos et al. (1988), Hu and Islam (1995), and Viterbo and Beljaars (1995). Important features of the model are highlighted below.

- The surface heat and moisture budgets are represented by two partial differential equations (assuming snow free ground). The total soil depth, number of layers, and boundary conditions are chosen such that all relevant time scales, ranging from diurnal cycles to seasonal cycles, are adequately represented.
- The evaporation rate from the canopy and from the bare soil consists of three components: evaporation of water from the wetted canopy and soil, transpiration of soil water extracted by the root system, and evaporation from the bare soil.
- Soil hydraulic and thermal properties are characterized using Clapp and Hornberger (1978) formulations.

The soil heat and moisture transfer are described by classical diffusion equations. The top boundary conditions are obtained from solution of the surface moisture and energy balance equations while the heat and moisture flux from the bottom of the fourth layer is taken to be zero. The thermal diffusivity and moisture diffusivity are parameterized as a function of soil moisture and temperature (Clapp and Hornberger, 1978). There are four soil layers and the depths of the soil layers are taken in an approximate geometric relation ($D_1 = 7$ cm, $D_2 = 21$ cm, $D_3 = 72$ cm, and $D_4 = 189$ cm) as suggested by Deardorff (1978) and adopted by Viterbo and Beljaars (1995). It has been shown that four layers are sufficient to capture soil moisture dynamics from diurnal to seasonal cycles (Viterbo and Beljaars, 1995). The root zone is spread within the first three layers and it extends up to 100 cm. The fourth layer extends between 100 and 289 cm with no root zone.

The land surface parameterization used in this study is guided by the concern to capture principal

Table 1
Parameters used in the land surface model

θ_{sat}, soil moisture at saturation ($m^3\ m^{-3}$)	0.47
θ_{cap} soil moisture at field capacity ($m^3\ m^{-3}$)	0.32
θ_{pwp} soil moisture at permanent wilting point ($m^3\ m^{-3}$)	0.17
Ψ_{sat}, matric potential at saturation (m)	− 0.34
γ_{sat}, hydraulic conductivity at saturation, ($m\ s^{-1}$)	4.57×10^{-4}
a, Clapp and Hornberger soil parameter	3.80
b, Clapp and Hornberger soil parameter	6.04
L_f, leaf area index	4

physical mechanisms through a minimum number of parameters. In representing the subsurface hydrology and evaporation, three processes appear important: first, a mechanism is necessary to get precipitation partitioned into runoff and infiltration; second, a storage is necessary to account for several weeks of evaporation without rain; third, seasonal and interannual memory of soil moisture anomalies need to be represented through a deep reservoir (e.g. Yang et al., 1995; Beljaars and Viterbo 1994). Yang et al. (1995) found that 'the equilibrated surface heat fluxes are extremely weakly dependent on the thickness of soil layer below the root zone, despite the strong relationship between spin-up time and the thickness.' Our experiments with one and two-layer models have shown similar results (Arendt et al., 1996). Viterbo and Beljaars (1995) found that two-layer soil moisture model, with average soil moisture values from the FIFE site and no drainage at the bottom of the layer, would give a time scale of about a week. As the influences of the soil moisture content below the root zone on near surface atmospheric variables are negligible, in mesoscale models and in four-dimensional data assimilation system, soil layer thickness below the root zone can be set to small values or even zero to ensure a short spin-up time (Yang et al., 1995). It is important, however, to note that the thickness of the deep layer would become important for long-range climate projections. Thus, it is essential to differentiate between 'weather' and 'climate' integrations. For mesoscale weather integrations (several days), it appears that two-layer soil moisture model would be adequate. A two-layer soil moisture would capture two of the three subsurface moisture transfer mechanisms discussed earlier. Extensive comparison with HAPEX–MOBILHY dataset with a two-layer soil moisture model and parameterized canopy layer shows that the model reproduces a realistic partitioning of energy over the forest and the crops (Noilhan et al., 1991).

To describe the third process, seasonal and interannual memory of soil moisture anomaly, additional two layers are included in our model. These layers are important for longer time scale climate simulations and may not play a significant role for mesoscale simulations. In choosing the total soil depth and spatial discretization, careful considerations were given to ensure that time scales relevant to weather and climate scale simulations are adequately captured with a parsimonious set of parameters without a significant sacrifice in numerical accuracy. Warrilow et al. (1986) have shown that four layers are adequate for representing time scales from one day to a year.

To parameterize sensible and latent heat fluxes, we use transfer coefficients or resistances between the surface and the lowest atmospheric model level expressed as a function of the Obukhov Length (Beljaars and Viterbo, 1994). Advantages of using the Obukhov Length instead of a simpler formulation in terms of Richardson Number (Louis, 1979) are discussed in Beljaars and Viterbo (1994). We will take the roughness length for heat equal to that for moisture. The evaporation rate from the soil-canopy system consists of evaporation of water from the wetted canopy and soil E_{WC}, transpiration of soil water extracted by the root system E_{tr}, and evaporation from the bare soil E_g. These three components of soil-canopy evaporation are estimated following Noilhan and Planton (1989) and Viterbo and Beljaars (1995). Table 1 provides a list of model parameters used in this study.

2.2. Description of data and model validation

In 1987, a large field experiment was launched on the Kansas Prairie (39°03′N and 96°32′W), known as the First ISLSCP FIFE. The experiment was centered on a 15×15 km area. A site-averaged data set for this experiment was quality controlled and edited by Betts and Ball (1992), and updated in Betts and Ball (1998). This is perhaps one of the most well-studied and reliable data sets suitable for a systematic analysis of soil moisture assimilation within a land surface model. This average data set has been useful for various

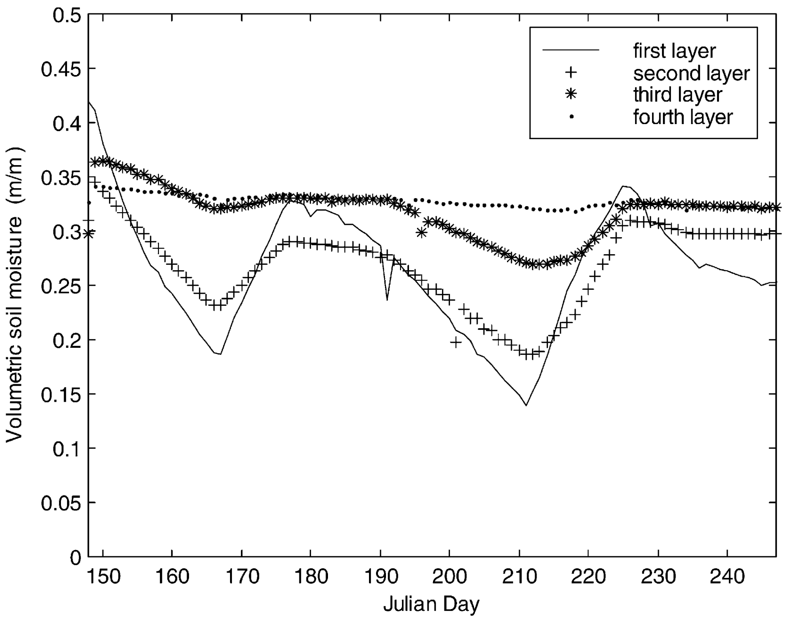

Fig. 1. Observed soil moisture for four layers from May 27 to Oct 15, 1987 for the FIFE 1987.

land surface model development, calibration, and validation (e.g. Viterbo and Beljaars, 1995; Chen et al., 1996). For a detailed description of this data set we refer to Betts et al. (1993) and Betts and Ball (1998). For this study, we will use this site-average data set for the period between May 27 and Oct 15, 1987.

During this period, all atmospheric forcing data needed for the land surface model are available in terms of 30 min averaged time series, which consist of air temperature, atmospheric pressure, precipitation rate, wind speed in two horizontal directions, mixing ratio, incident solar radiation and downward long wave radiation. All variables were measured at (or converted to) a reference level of 2 m. Surface flux measurements were made by both eddy correlation and Bowen ratio methods. Soil moisture was systematically measured at a large number of sites by two methods: gravimetric method for the near surface layers and neutron probe method for depths up to 2 m. Gravimetric soil moisture were taken from 0 to 5 and 5 to 10 cm, then converted to volumetric units. In deeper layers, volumetric soil moisture profile was taken from neutron probe measurements. Therefore, all soil moisture data here are expressed in percentage. Fig. 1 shows the observed soil moisture for four layers for the FIFE average data set. The surface soil moisture shows the largest amplitude of variability while the variability decreases as we go to deeper layers. The surface soil moisture responds to changes in precipitation, evaporation, and redistribution more rapidly than any other layers. Viterbo and Beljaars (1995) have also pointed out that the deeper the layer is the longer the response time. For instance, in this case, the surface soil moisture goes through a series of wetting and drying cycles while the fourth layer essentially fluctuates around the field capacity.

Our use of the FIFE near surface gravimetric measurements of soil moisture as a surrogate of remote sensing measurements was motivated by the availability of a continuous data set of soil moisture for an extended period of time. In addition to soil moisture, as indicated earlier, several other forcing (e.g. radiative flux, precipitation, air temperature, etc.) and response (e.g. surface fluxes) variables are also available for the FIFE 1987 experiment.

We have performed a detailed validation of this land surface model using the FIFE data (Li and Islam, 1999). We highlight some of the findings of model validation here. The soil moisture for the first two layers is predicted well by the model. There appears to be a slight underestimation bias for the deeper layers. The latent heat flux is predicted well with a correlation coefficient of 0.92, a positive bias of 10.3 W m^{-2}, and a root mean square error of 20.87 W m^{-2}. Sensible heat flux, on the contrary, has a bias of −22.14 W m^{-2}, correlation coefficient of 0.65, and root mean square error of 31.06 W m^{-2}. Viterbo and Beljaars (1995) have also done an extensive validation for this model for a range of surface and climate conditions including the FIFE in the United States, Cabauw in the Netherlands, and ARME in the central Amazonia. A version of this land surface model is currently used as a host land surface model within the ECMWF model.

3. Methodology

We will use the FIFE data and a four-layer land surface model to address the questions identified in Section 1. The near surface soil moisture goes through successive wetting and drying cycles in response to precipitation, evaporation, and redistribution. To understand the relationship between the near surface soil moisture and the soil moisture profile, it is important to examine such a relationship for various soil moisture conditions (e.g. drying to wetting, wetting to drying, etc.). We define a full cycle such that surface soil moisture goes through a complete succession of drying and wetting while a half cycle is referred to as either the drying or the wetting phase. It is understood that these cycles are not exactly identical in terms of phase or amplitudes. Nevertheless, it gives us a framework to analyze response of the surface soil moisture and the soil moisture profile under different conditions. Based on this definition, we can identify three full cycles from the FIFE 1987 data: May 27–June 25, June 25–Aug 11, June 15–July 29; and three half cycles: May 27–June 15, June 15–June 25, June 25–July 09. These six periods range from 11 days (June 15–June 25) to 48 days (June 25–Aug 11), and includes various combinations of wetting and drying sequences.

One way to retrieve the soil moisture profile is to find the optimal estimates of surface soil moisture by inverting a land surface model and assuming an optimization criteria (Calvet et al., 1998). As we pointed out earlier, this is an attractive proposition. If it is valid for a wide range of surface and atmospheric conditions then one will be able to use remotely sensed surface soil moisture and a land surface model to estimate the soil moisture profile. To examine the suitability of this retrieval methodology, we will examine the correlation between the soil moisture profile and the surface soil moisture and for three full and half cycles of soil moisture evolution defined earlier. We will simulate these full and half cycles for a range of deeper layer(s) soil water content, namely the second layer soil moisture (W_2) and the third layer soil moisture (W_3). We note here that the layers are defined in terms of depth as D_1, D_2, D_3 and D_4 while the corresponding soil moisture for each layer is defined as W_g, W_2, W_3 and W_4. In these simulations, we will vary the range of initial second and third layer soil moisture between the wilting point (0.15) and the saturation point (0.45) with an interval of 0.05. This range is chosen based on the averaged soil property of the FIFE site (Table 1). In reality, W_2 and W_3 are likely to have different initial values for each simulation. It is not clear, however, how to initialize these two layers differently. Consequently, we have decided to assign the same initial values for W_2 and W_3. The surface soil moisture, W_g, is initialized with the exact observation depending on when the simulation starts. Given the length of the full and half cycles and the response time of various soil layers, we have decided to keep the initial soil moisture for the fourth layer to be a constant. A quick look at Fig. 1 suggests that there is a very little change in the fourth layer soil moisture for the entire observation period and it fluctuates around the field capacity value. Consequently, in all our simulations, the initial value for the fourth layer soil moisture is kept at the field capacity.

For six sets of experiments described earlier, the first layer soil moisture W_g, sensible heat flux H, and latent heat flux LE are simulated with different initialization of W_2 and W_3. To quantify the similarities and differences among these simulations, we use normalized root mean square error (NRMSE) as a metric of comparison. It is defined as the ratio of the root mean square error and observed standard deviation. This normalized metric would allow us to compare response of different variables with highly contrasting range and units for soil moisture and surface fluxes.

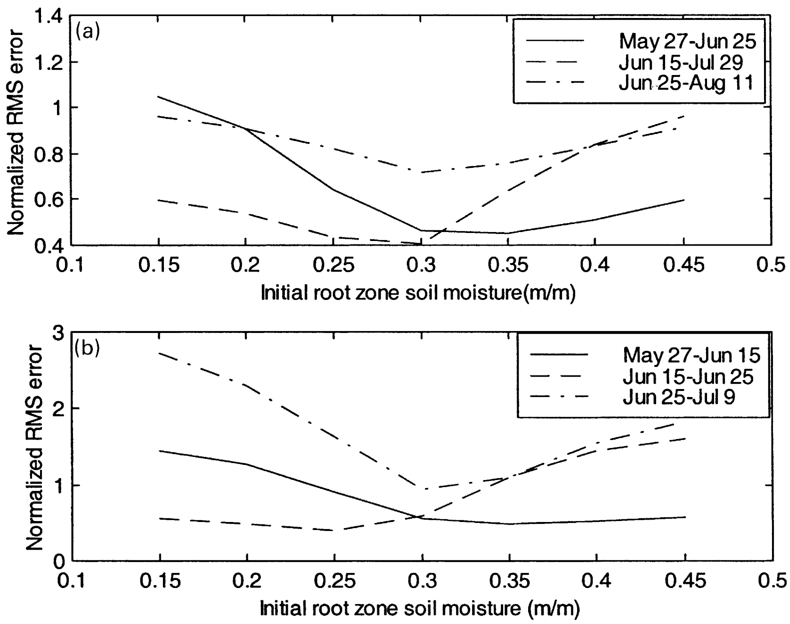

Fig. 2. (a) Normalized root mean square error (NRMSE) of estimated daily surface soil moisture for a range of deeper layer(s) soil moisture for three full cycles; (b) Similar to (a) but for half cycles.

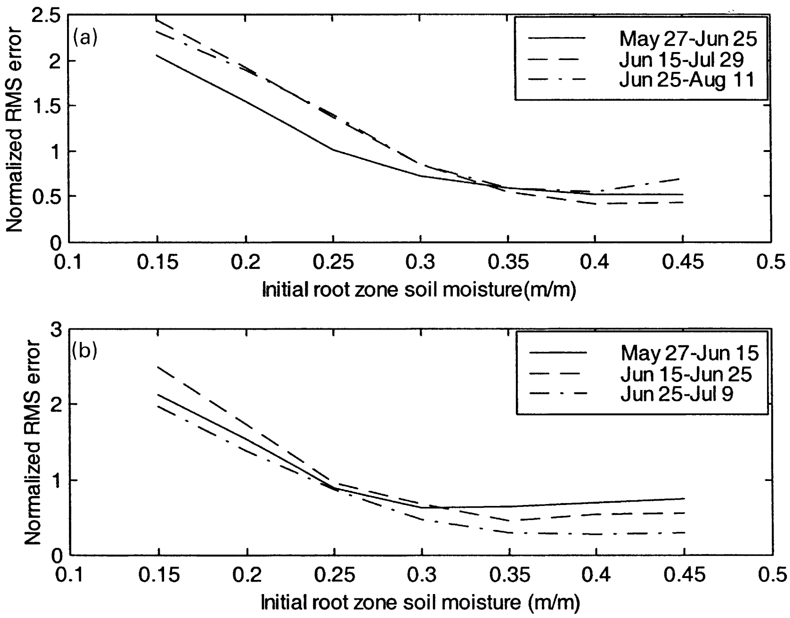

Fig. 3. (a) Similar to Fig. 2(a), but for daily latent heat flux. (b) Similar to (a), but for half cycles.

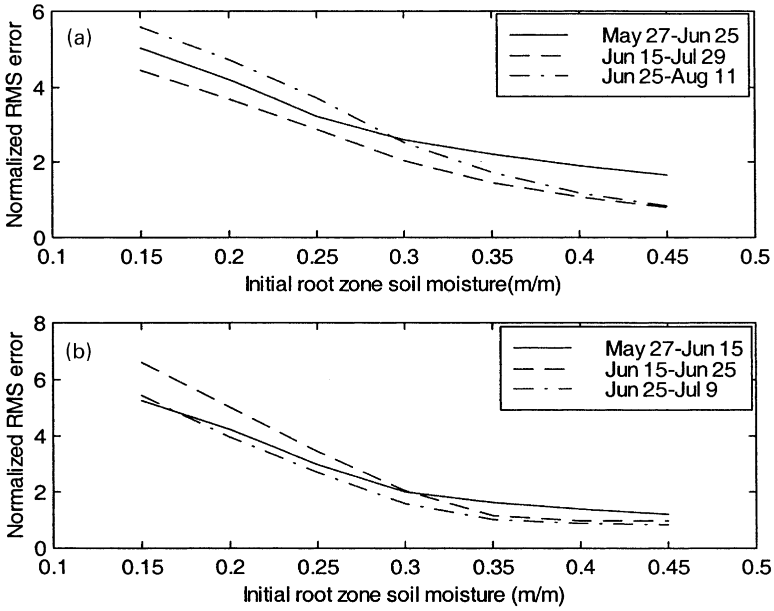

Fig. 4. (a) Similar to Fig. 2(a), but for daily sensible heat flux. (b) Similar to (a), but for half cycles.

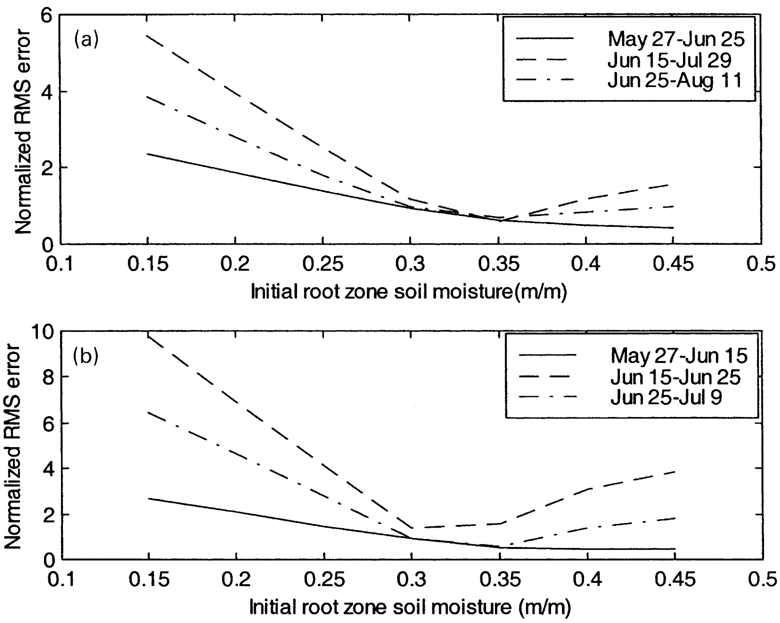

Fig. 5. (a) Similar to Fig. 2(a), but for daily integrated root zone soil moisture. (b) Similar to (a), but for half cycles.

Table 2
Comparison of profile integrated soil moisture for different cycles and initializations

Profile integrated soil water (cm)	Cycles 1 and 2	Cycles 3 and 4	Cycles 5 and 6
Observed	30.834	29.311	28.812
Initialize with surface soil moisture	42.000	32.800	18.600
Initialize with field capacity	30.000	30.000	30.000

4. Results

4.1. Relationship between the soil moisture profile and surface soil moisture and fluxes

Fig. 2 shows the NRMSE of surface soil moisture (i.e. first layer) estimation for a range of second and third layer soil moisture initialization using the six cycles of soil moisture evolution defined earlier. Surface soil moisture shows a high degree of sensitivity to the initialization of deeper layer soil water content. The NRMSE estimated for different initialization differs from each other by a factor of as large as three. It appears that the larger the deviation of initialization from the observed surface soil moisture, the larger the NRMSE. For example, for simulations of May 27–June 25 and May 27–June 15, $(W_g)_0 = 0.420$, and initialization of $(W_2)_0 = (W_3)_0 = 0.15$ gives the largest NRMSE; for simulation of Jun 15–Jul 29 and Jun 15–Jun 25, $(W_g)_0 = 0.186$, and $(W_2)_0 = (W_3)_0 = 0.45$ produces the maximum NRMSE.

The NRMSE is usually smaller for the full cycles (Fig. 2(a)) compared to the half cycles (Fig. 2(b)). However, there appears to be a minima at $(W_2)_0 = (W_3)_0 = 0.30$, which is approximately the field capacity, for all the cases examined irrespective of the starting point or the cycle length.

Similar to the surface soil moisture, the estimation of surface fluxes also shows great sensitivity to the initialization of deeper layer(s) soil moisture. But the nature of sensitivity is different from that of surface soil moisture. The deeper layer soil moisture initializations appear to reduce the estimation error in surface fluxes as we progressively increase the initial values of deeper layer soil moisture till the field capacity irrespective of the initial surface soil moisture. When the initial values of W_2 and W_3 are equal to or greater than the field capacity, the NRMSE shows little sensitivity to latent heat flux (Fig. 3). However, the NRMSE for sensible heat flux continues to go down for increasing values of initial deeper layer soil moisture (Fig. 4). The sensitivity of profile integrated soil moisture is similar to those of latent heat flux (Fig. 5, Table 2). An implication of this is that latent heat flux is more or less proportional to integrated soil water in the deeper layers.

Analysis of Figs. 2–5 suggests that estimation of surface soil moisture, integrated profile soil water content, sensible heat flux, and latent heat flux are quite sensitive to initialization of deeper layer(s) soil moisture for typical wetting and drying cycles spanning from several days to several weeks. However, the degree and characteristics of these sensitivities are different for different variables. In particular, if one chooses the initial soil moisture profile that optimizes the NRMSE with respect to surface soil moisture, it may not always lead to optimal estimation of surface fluxes. Since surface fluxes, especially latent heat flux, is closely related to integrated soil moisture. It appears that a decoupling between the surface and the deeper layer soil moisture proposed by Capehart and Carlson (1997) could partly explain the differences in sensitivity for surface soil moisture and surface fluxes.

For the FIFE site, estimation of surface fluxes from an optimal choice of deeper layer soil moisture is further complicated by the presence of dense vegetation cover. The FIFE site is covered with tall grass with an approximate fractional vegetation cover of 85%. As a consequence, much of the water for evapotranspiration is derived from root zone extraction. We separate the three components (evaporation of water from the wetted canopy and soil, transpiration of soil water extracted by the root system, and evaporation from the bare soil) of the estimated evapotranspiration for the FIFE site and find that the extraction of the root zone account for approximately 90% of the total evapotranspiration. Effects of root zone distribution on the estimation error are discussed later.

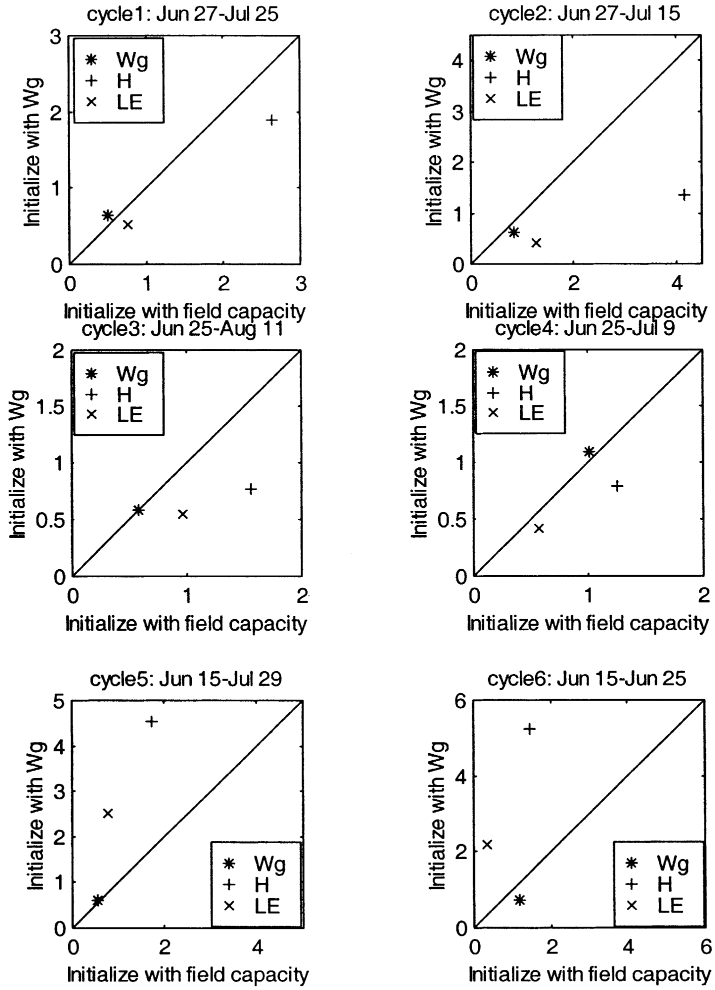

Fig. 6. Normalized root mean square error (NRMSE) of estimated daily surface soil moisture, daily sensible heat flux, and daily latent heat flux by initializing the soil moisture profile based on remotely sensed surface soil moisture (W_g) against those from initialization of soil moisture profile at field capacity.

4.2. Effects of soil moisture profile initialization based on remotely sensed soil moisture

The above analysis suggests that the inversion of a land surface model using optimal choice of initial deeper layer soil moisture is not likely to produce an accurate retrieval of soil moisture profile and accurate estimation of surface fluxes, specially for drier initial surface soil moisture conditions. Now, we will explore the possibility of extracting the soil moisture profile based on remotely sensed surface soil moisture. Here, the observed surface soil moisture is taken as a surrogate for remotely sensed soil moisture. We will compare these estimates based on deeper layer soil moisture initialization at its field capacity because the analysis from Section 4.1 suggests that, irrespective of surface and atmospheric conditions, field capacity appears to provide the most consistent and optimal estimates of the profile soil moisture. Our objective in this section is to explore whether it is possible to further reduce the estimation error of soil moisture profile based on remotely sensed surface soil moisture.

We note here the disparity in scales between the remotely sensed surface soil moisture (measured with a scale of hundreds of meters) and deeper layer soil moisture (measured at a point). Usually, most biophysically based soil–vegetation–atmosphere transfer models are assumed to be scale-invariant with respect to the boundary conditions of topography, vegetation, and soil moisture. Sellers et al. (1997) have performed a systematic study to ascertain the validity of this assumption using FIFE-89 dataset. They have divided the FIFE domain into pixels with 30×30 m spatial resolution, each of these pixels were assigned topographic, vegetation, and soil parameters from satellite and in situ observations. Sellers et al. (1997) conclude that simple averages of topography and vegetation parameters can be used to calculate surface fluxes over a range of spatial scales, from meters to several kilometers, for grassland areas with moderate topography. These results suggest that, at least for areas like the FIFE domain, it would be reasonable to assume scale invariant boundary conditions of topography, vegetation, and soil parameters within the context of this study.

To explore the possibility of further reducing the estimation error of soil moisture profile based on remotely sensed surface soil moisture, we perform six simulations: three full cycles and three half cycles defined before. In these simulations, initial value of soil moisture at each layer is either set to the remotely sensed surface soil moisture or to a uniform field capacity. If there is a decoupling between the surface and deeper layer soil moisture, cycles with high initial surface soil moisture is expected to show minimal effect of decoupling. While cycles with drier initial surface soil moisture is expected to show pronounced effects of decoupling.

To evaluate the influence of decoupling, the NRMSE is calculated for the surface soil moisture, sensible heat flux, and latent heat flux for these six simulations. For each cycle, the NRMSE obtained with the initial profile at the field capacity are plotted against those obtained with the profile initialized with remotely sensed soil moisture (Fig. 6).

If there is a decoupling between the surface and deeper layer soil moisture, one can argue that cycles with high initial surface soil moisture, such as cycles starting on May 27 and June 25 (cycles 1–4), will show minimal effect of decoupling. Consequently, these cycles will be better initialized from remote sensing of surface soil moisture compared to those initialized based on uniform field capacity. Fig. 6 (cycles 1–4) clearly demonstrates this point. While cycles with drier initial surface soil moisture, cycles starting on June 15 (cycles 5 and 6), show pronounced effects of decoupling. An initialization based on field capacity yields better estimates of surface soil moisture and fluxes for these cycles (Fig. 6: cycles 5 and 6).

It appears that constant vertical profile based on surface soil moisture overinitializes the integrated water in deeper layers for cycles 1–4 and underinitializes in cycles 5 and 6. In contrast, vertical profile based on field capacity underinitializes integrated soil moisture for cycles 1–4 and overinitializes for cycles 5 and 6 (Table 1). Based on these results, one may argue that overinitialization of the integrated soil water in deeper layers leads to better estimation of surface fluxes partitioning. One of the possible reasons may be attributed to the root zone distribution used in the model. In this model formulation, root zone is uniformly distributed in the first three layers, i.e. $R_1 = R_2 = R_3 = 0.33$ (Viterbo and Beljaars, 1995). Since the soil layer depths follow a geometric series, root zone density exponentially decrease with depth. Such a distribution of root profile, however, may not be appropriate for the FIFE site which is dominated by tall grass. Also, the surface layer is much thinner than the second and third layer, and the average soil moisture in the first layer is lower than that of the second and third layers. Consequently, less water is available in the first layer compared with the other two layers for root extraction. Therefore, a uniform distribution of root zone, as used in this model, would lead to the underestimation of root extraction. It appears that overinitialization of second and third layer soil moisture attempts to counteract this underestimation and consequently leads to lower estimation error in surface fluxes.

Further analysis suggests that a reduction of root distribution in the first layer and increase of root distribution in deeper layers leads to significant reduction in RMS error for estimated sensible and latent fluxes. For instance, we assume that the root zone distribution in the soil is proportional to the depth of each layer: $R_1 = 0.07$, $R_2 = 0.21$, and $R_3 = 0.72$. For the May 27–Jun 25 simulation, W_2 and W_3 initialized at the field capacity, the root mean square errors are 15.98 and 23.27 W m^{-2} for latent heat flux and sensible heat flux, respectively. These errors are significantly smaller compared to those from uniformly distributed root zone, 25.21 and 50.89 W m^{-2} for latent and sensible heat fluxes, respectively. We must note, however, our assumption of a geometric root zone distribution has no direct physical basis and it was chosen to demonstrate the difficulties associated with the retrieval of the deeper layer soil moisture from remotely sensed soil moisture through a model inversion technique.

5. Conclusions

An accurate estimation of soil moisture profile is necessary for various hydrometeorological, ecological, and biogeochemical modeling and applications. Remote sensing techniques are increasingly being used for monitoring soil moisture conditions over large areas. The shallow moisture sensing depth of passive microwave sensors, however, limits the use of remotely sensed soil moisture for many land–atmosphere interaction, ecosystem dynamics, and biogeochemical cycle studies.

In this study, we examine the feasibility of retrieving the soil moisture profile from surface measurements through a model inversion technique, suggested by Calvet et al. (1998). We also explore the adequacy of partitioning of surface fluxes as a function of retrieved soil moisture profile. We use a four-layer land surface model and observed data sets from FIFE 1987 to address these issues.

To evaluate the adequacy of retrieving the soil moisture profile from surface measurements, we examine the relationship between the deeper layer soil moisture and surface soil moisture, surface fluxes, and column integrated soil moisture for various surface and atmospheric conditions. Surface soil moisture shows a high degree of sensitivity to the initialization of deeper layer soil water content. The normalized root mean square error is usually smaller for the full cycles compared to the half cycles for various initial conditions. Similar to the surface soil moisture, the estimation of surface fluxes also shows great sensitivity to the initialization of deeper layer soil moisture. But the characteristics of these sensitivities are different from those of surface soil moisture. The sensitivity of profile integrated soil moisture, however, is similar to that of latent heat flux suggesting that latent heat flux is more or less proportional to integrated soil water in the deeper layers. It appears that if one chooses the initial soil moisture profile that optimizes normalized root mean square error with respect to surface soil moisture, it may not lead to optimal estimation of surface fluxes. These results suggest that the inversion of a land surface model with an optimal (in terms of minimum root mean square error) initial soil moisture profile may not always lead to accurate retrieval of deeper layer soil moisture and correct partitioning of surface fluxes.

We show that the accuracy of deeper layer soil moisture retrieval from surface measurements depends strongly on the initial surface soil moisture conditions. For wetter surface soil moisture conditions, an initialization based on remotely sensed surface soil moisture appears to be adequate for the retrieval of deeper layer soil moisture. For drier surface conditions, however, a decoupling of surface and deeper layer soil moisture is triggered and an initialization based on surface moisture would lead to larger error. These results are consistent with those of Capehart and Carlson (1997). They argued that the drying proceeds at about the same rate for surface and deeper layers when the initial soil water content is above some threshold. Below this threshold, the drying is enhanced near the surface and the deeper layers get gradually decoupled from the surface due to the reduction in near surface hydraulic conductivity. We must note, however, that such a decoupling between the surface and the lower layer soil moisture is likely to be dampened by the presence of vegetation and plants.

Results of this study must be interpreted with caution because it utilizes surrogate microwave measurements of soil moisture. In reality, microwave provides instantaneous measurements of soil moisture. Thus, additional experiments are needed with actual measurements of surface soil moisture from remote sensing to confirm and extend the findings of this research. We also note the disparity in scales between the scale of remote sensors (hundreds of meters) and the in situ observations of deeper layer soil moisture measurements. An assumption of scale invariance for the initial boundary conditions for topography and vegetations seems appropriate for a relatively homogeneous domain like the FIFE site.

More experiments, however, are needed with different surface conditions to generalize these results. Our preliminary analysis evaluates the merits of a model inversion technique to estimate soil moisture profile at a point. To characterize the space–time structure of soil moisture profile and surface fluxes partitioning, we need to extend the above methodology over large areas. This will require a distributed land surface model which can incorporate spatially variable atmospheric forcing and surface parameters into the model formulations. The influence of root zone and root density distribution on the retrieval of the profile soil moisture estimation also needs further research.

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