One-Dimensional Soil Moisture Profile Retrieval by Assimilation of Near-Surface Measurements: A Simplified Soil Moisture Model and Field Application

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ABSTRACT

The Kalman filter assimilation technique is applied to a simplified soil moisture model for retrieval of the soil moisture profile from near-surface soil moisture measurements. First, the simplified soil moisture model is developed, based on an approximation to the Buckingham–Darcy equation. This model is then used in a 12-month one-dimensional field application, with updating at 1-, 5-, 10-, and 20-day intervals. The data used are for the Nerrigundah field site, New South Wales, Australia. This study has identified (i) the importance of knowing the depth over which the near-surface soil moisture measurements are representative (i.e., observation depth), (ii) soil porosity and residual soil moisture content as the most important soil parameters for correct retrieval of the soil moisture profile, (iii) the importance of a soil moisture model that represents the dominant soil physical processes correctly, and (iv) an appropriate forecasting model as far more important than the temporal resolution of near-surface soil moisture measurements. Although the soil moisture model developed here is a good approximation to the Richards equation, it requires a root water uptake term or calibration to an extreme drying event to model extremely dry periods at the field site correctly.

1. Introduction

An ability to retrieve the soil moisture profile by assimilation of near-surface soil moisture measurements (such as would be obtained from remote sensing) in a soil moisture model has received an increasing amount of attention over the past decade. Recent studies (Houser et al. 1998; Walker et al. 2001) have suggested that statistical assimilation techniques such as the Kalman filter, through their ability to modify directly the soil moisture estimates of deeper soil layers, show the most promise in this application. However, the majority of assimilation studies that have applied such techniques have been limited to synthetic desktop studies and/or short time periods, such as the 8-day study of Galantowicz et al. (1999).

To make a progression from the more common one-dimensional desktop studies using synthetic data to realistic catchment-scale field applications, we must first illustrate this potential through long-term one-dimensional studies using field data. These studies need to be developed in such a way that they have relevance to studies at the catchment scale. Moreover, the soil moisture model used must be characteristic of the model that will be used by the catchment-scale studies. One of the limitations in undertaking such studies is the lack of good-quality soil moisture and atmospheric forcing data over longer time periods that have application to one-dimensional models. This paper presents a computationally efficient conceptual soil moisture model that has relevance in both one- and three-dimensional assimilation studies. Moreover, an appropriate dataset for a one-dimensional application is presented, and the results from such an application are discussed. This dataset is for the Nerrigundah experimental catchment, located in a temperate region of eastern Australia.

2. Simplified soil moisture model

To apply the soil moisture profile retrieval algorithm established by Walker et al. (2001) to a one-dimensional field application, with the vision of extending the methodology to the catchment scale, a computationally efficient soil moisture model suitable for near-surface soil moisture data assimilation in a shallow soil catchment of temperate eastern Australia was required. This section of the paper describes the development of such a model.

a. Model requirements

The requirements for a soil moisture profile model that can be applied to both one-dimensional and spatially distributed applications while being suitable for

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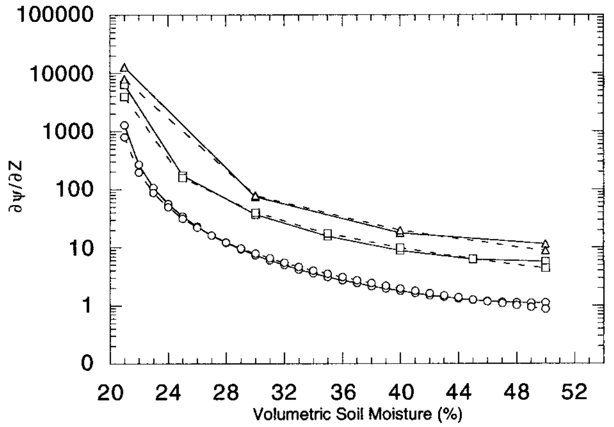


FIG. 1. Comparison of the vertical distribution factor (dashed line) with $\partial\psi/\partial Z$ from the van Genuchten (1980) relationship (solid line) for three different $\Delta\theta$ with a given separation Δz of 10 cm: 1% v/v (circle), 5% v/v (square), and 10% v/v (triangle). Here v/v is volume of water to volume of soil.

use within the framework of the Kalman filter assimilation scheme are as follows.

1) Describe the spatial distribution and temporal variation of soil moisture profiles, not just profile storage, while maintaining simplicity and computational feasibility. The need for soil moisture variation with depth is to have a thin near-surface layer that is compatible with the soil moisture observation depth and to have correlation between this near-surface layer and deeper soil layers.
2) Allow for both upward redistribution during drying events and gravity drainage during wetting events without having an implicit assumption about a water table at some depth, while maintaining lateral redistribution in a catchment application.
3) Have a spatial discretization that is compatible (i.e., grid-based rather than stream tubes) with the grid-based remote sensing observations of near-surface soil moisture.
4) Forecast soil moisture as a linear function of the soil moisture at the previous time step and be as close to a linear representation of the model physics as possible, that is, model volumetric soil moisture content as the dependent state rather than matric head (Walker et al. 2001). This is required to satisfy the underlying linearity assumption of the Kalman filter in forecasting of the soil moisture covariance matrix and hence to ensure more stable updating of the soil moisture forecasts.
5) Be in a form that will allow correlations to build up between soil layers (and grid elements). This is required to facilitate the updating of soil moisture content at deeper depths in the soil profile. Using the Kalman filter assimilation scheme, updating only occurs if the forecast covariance matrix of system-states indicates there is a correlation with the near-surface soil moisture observations. These correlations are generated if the change in soil moisture content of a soil layer is a function of the soil moisture content in the adjacent soil layers.

TABLE 1. Soil parameters used for evaluation of the vertical distribution factor and $\partial\psi/\partial Z$ in Fig. 1.

Residual soil moisture content θ_r	20% v/v
Soil porosity ϕ	54% v/v
van Genuchten parameter η	0.0008 mm^{-1}
van Genuchten parameter n	1.8
Soil discretization Δz	100 mm
Max gradient parameter MGRAD	270 mm

b. *Applicability of existing models*

When choosing a hydrologic model it is necessary to identify the key processes that are active in the catchment under consideration and to ensure that they are satisfactorily represented by the model (Hughes 1994). For example, catchments located in semiarid regions typically have shallow soils overlying an impermeable layer of bedrock, resulting in no permanent water table (but a transient water table may form during wet periods, particularly in the convergent zones) and essentially zero moisture flux between the soil and bedrock. Moreover, vertical rise of soil moisture from deeper layers to the surface during extended periods of exfiltration is an important process that must be captured by the hydrologic model. For example, the Nerrigundah experimental catchment (where the data were collected for the field application discussed later in this paper) has thin soil overlying very low permeability sandstone and exhibits vertical rise of soil moisture from deeper layers to the soil surface. Although many soils have significant crack or other macropore systems (Kirkby 1985), such systems were not identified in the Nerrigundah catchment and consequently will not be modeled.

A limitation of many existing hydrologic models is their emphasis on runoff estimation (e.g., Beven and Kirkby 1979; Boughton 1983; Moore and Grayson 1991; Wood et al. 1992; Ottlé and Vidal-Madjar 1994) at the expense of a realistic representation of the soil moisture profile. Furthermore, those models that account for soil moisture more explicitly often have restrictive assumptions (which can be problematic under certain situations), such as

- a water table exists for the lower boundary condition (e.g., Famiglietti et al. 1992; Famiglietti and Wood 1994a,b) or the water table is very deep (e.g., Rao et al. 1990; Lakshmi et al. 1997),
- there is no lateral redistribution between grid elements (e.g., Groves 1989; Ottlé et al. 1989; Capehart and Carlson 1994),
- all rainfall enters the soil until saturation (e.g., Wigmosta et al. 1994),
- soil moisture can be modeled with only two soil layers (e.g., Beven and Kirkby 1979; Ottlé et al. 1989; Liang

TABLE 2. Soil parameters used in evaluation of the conceptual model.

Total soil depth	1000 mm
No. of layers	30
Soil type	Clay loam
Saturated hydraulic conductivity K_s	20.8 mm day^{-1}
Soil porosity ϕ	54% vv
Residual soil moisture content θ_r	20% v/v
van Genuchten parameter η	0.0008 mm^{-1}
van Genuchten parameter n	1.8
Max gradient parameter MGRAD	280 mm
Initial condition	−500 mm matric head

et al. 1994; Hughes and Sami 1994; Wigmosta et al. 1994; Lakshmi et al. 1997),

- there is a constant soil moisture with depth at the start of infiltration and exfiltration periods (e.g., Eagleson 1978; Groves 1989), or
- there is gravity drainage but no upward redistribution to recharge the near-surface layer(s) (e.g., Beven and Kirkby 1979; Cabral et al. 1992; Liang et al. 1994; Wigmosta et al. 1994).

Of those models that do account for upward redistribution, which has been shown by Liang et al. (1996) to be important in achieving realistic results for low soil moisture contents, the Richards equation has generally been applied with the assumption that it is applicable for a coarse vertical discretization (e.g., Liang et al. 1996; Lakshmi et al. 1997). However, for accurate solution to the Richards equation, it is necessary to use a fine vertical discretization. In addition, discretization of the horizontal model domain is often not compatible with the observation domain (e.g., Moore and Grayson 1991) because the soil moisture is not modeled on a regular grid or is not comparable with the observations (e.g., Beven and Kirkby 1979; Wood et al. 1992; Hughes and Sami 1994) because the soil moisture distribution is modeled statistically.

To satisfy the soil moisture profile retrieval algorithm forecasting model requirements outlined above and to overcome the limiting assumptions and restrictions of existing models, a computationally efficient conceptual model of soil moisture has been developed. Although the computational requirements of this model would not be much different to those of the Richards-equation model with a coarse discretization, this is a conceptual model, rather than a theoretical model that was developed for a fine model discretization, and as such may be used for a coarse discretization without violating the key assumptions of the model. This is not intended to be the next state-of-the-art model for soil moisture data assimilation but rather a model that satisfies the requirements set out in the foregoing discussion, with the view that it will be used in a follow-on catchment-scale assimilation study.

c. Model development

Unsaturated flow through porous media can be described by the Buckingham–Darcy equation as

$$Q = K\nabla(\psi + z), \tag{1}$$

where Q is the volumetric flux of liquid water per unit area, K is the unsaturated hydraulic conductivity, ∇ is the gradient operator, ψ is the matric suction, and z is the elevation (positive downward).

The approach taken by our Approximate Buckingham-Darcy Equation for Moisture Estimation (ABDOMEN) model has been to solve an approximate form of the Buckingham-Darcy equation using an implicit solver. The Buckingham-Darcy equation for vertical flux Q_V (positive downward) can be written as

$$Q_V = K\frac{\partial\psi}{\partial Z} + K\frac{\partial z}{\partial Z}. \tag{2}$$

The first right-hand-side term in this equation is a matric suction term, which tends to move soil moisture toward areas of greater matric suction (lower soil moisture), and the second right-hand-side term accounts for gravity drainage. Thus, soil moisture can move upward against gravity during an exfiltration event if the matric suction term is greater than the gravity drainage term. Likewise, during an infiltration event, the soil moisture wetting front can move downward faster than for gravity drainage.

1) A CONCEPTUAL SOIL MOISTURE FLUX EQUATION

Accurate solution of the Buckingham–Darcy (Richards) equation requires a fine spatial discretization of the model domain and a large computational effort. In addition, the Buckingham–Darcy equation requires knowledge of the ψ–θ relationship (where θ is the volumetric soil moisture content), adding complexity to the model. Therefore, a simplified version of (2) is proposed:

TABLE 3. Calibrated soil parameters for the simplified one-dimensional soil moisture model from connector TDR soil moisture data.

Layer	Thickness (mm)	Horizon	K_s (mm h^{-1})	ϕ (% v/v)	θ_r (% v/v)	n	MGRAD (mm)
1	10	A1	15	60	6	2.18	23
2	45	A1	15	60	6	2.18	23
3	68	A2	15	46	8	1.34	22
4	112	B1	3	42	12	2.19	50
5	225	B2	0.4	48	18	1.46	275

$$Q_V = K \times \mathrm{VDF} + K, \tag{3}$$

where VDF is a vertical distribution factor that can be used to describe the redistribution of soil moisture by matric suction (equivalent to $\nabla\psi$) without modeling matric suction directly.

An appropriate form for the distribution factor may be obtained by conceptually analyzing a series of limiting cases: uniform moisture profile, infiltration, and exfiltration. These limiting cases would indicate that the distribution factor should be (i) zero if adjacent elements have the same soil moisture content, (ii) positive if the upward element has a greater soil moisture content, (iii) negative if the downward element has a greater soil moisture content, and (iv) approach $\pm\infty$ if the difference in moisture content of adjacent elements is great (assuming uniform soil properties). Based on these observations, the following distribution factor, which is independent of model discretization and incorporates the matric-head nonlinearity with soil moisture content, is proposed [for a complete development see Walker (1999)]:

$$\mathrm{VDF} = \frac{\mathrm{MGRAD}}{\Delta Z}\left[\frac{1}{(\theta_{j+1/2} - \theta_r)^2}\right]\left(\frac{\theta_j - \theta_{j+1}}{\phi - \theta_r}\right), \tag{4}$$

where MGRAD is a maximum gradient parameter, ΔZ is the perpendicular distance between the midpoints of layers j and $j + 1$, θ_j is the volumetric soil moisture of layer j, $\theta_{j+1/2}$ is the average soil moisture for layer j and $j + 1$, ϕ is the soil porosity, and θ_r is the residual soil moisture content. Using this conceptualization, the final term is -1 when $\theta_j = \theta_r$ and $\theta_{j+1} = \phi$, $+1$ when $\theta_j = \phi$ and $\theta_{j+1} = \theta_r$, and 0 when $\theta_j = \theta_{j+1}$. MGRAD is then used to scale the distribution factor from $-\infty$ to $+\infty$, to be consistent with the conceptualization. Dividing the scaling factor MGRAD by the layer separation reduces VDF when the separation is increased. Multiplying by the nonlinearity (middle) term increases VDF for low soil moisture content and decreases VDF at high soil moisture content. This is in keeping with typical moisture retention relationships, which have a nonlinear dependence of matric suction with soil moisture content, particularly at low soil moisture contents.

A comparison of the VDF with $\partial\psi/\partial Z$ from the van Genuchten (1980) relationship is given in Fig. 1 using the typical soil parameters in Table 1, by calculating ψ for two soil moisture contents with a difference of $\Delta\theta$. This figure shows a very good comparison, with the exception of soil moisture values close to the residual soil moisture content and soil porosity values. Without the nonlinearity term in (4), the relationship would plot as a horizontal line on Fig. 1.

2) INHOMOGENEOUS VERTICAL DISTRIBUTION FACTOR

To account for spatial heterogeneity in soil properties (i.e., residual soil moisture content and soil porosity), the distribution factor in (4) can be written as

$$\mathrm{VDF} = \mathrm{GRAD}_{j+1/2}\left(\frac{\theta_j - \theta_{r_j}}{\phi_j - \theta_{r_j}} - \frac{\theta_{j+1} - \theta_{r_{j+1}}}{\phi_{j+1} - \theta_{r_{j+1}}}\right), \tag{5a}$$

where

$$\mathrm{GRAD}_{j+1/2} = \frac{0.5}{\Delta Z}\left[\frac{\mathrm{MGRAD}_j + \mathrm{MGRAD}_{j+1}}{(\theta_j - \theta_{r_j})^2 + (\theta_{j+1} - \theta_{r_{j+1}})^2}\right]. \tag{5b}$$

The difference between the distribution factors in (4) and (5) is the allowance for different residual soil moisture content, soil porosity, and/or maximum gradient parameter for each soil layer. Equation (5) reduces to (4) when adjacent layers have the same soil properties.

3) THE GLOBAL SOIL MOISTURE EQUATION

By substitution of the distribution factor from (5) into the conceptual soil moisture flux equation in (3), the conceptual soil moisture flux equation can be discretized for the vertical moisture flux:

$$\begin{aligned} Q_{V_j} = {} & \left[\frac{\mathrm{GRAD}_{j+1/2} \times K_{j+1/2}}{(\phi_j - \theta_{r_j})}, -\frac{\mathrm{GRAD}_{j+1/2} \times K_{j+1/2}}{(\phi_{j+1} - \theta_{r_{j+1}})}\right]\begin{Bmatrix} \theta_j \\ \theta_{j+1} \end{Bmatrix} \\ & + \left[K_{j+1/2} - \mathrm{GRAD}_{j+1/2} \right. \\ & \left. \times K_{j+1/2}\left(\frac{\theta_{r_j}}{\phi_j - \theta_{r_j}} + \frac{\theta_{r_{j+1}}}{\phi_{j+1} - \theta_{r_{j+1}}}\right)\right], \end{aligned} \tag{6a}$$

where

$$K_{j+1/2} = (K_j + K_{j+1})/2. \tag{6b}$$

The model parameters K and GRAD are estimated from the soil moisture contents of the current time step. By applying the same methodology, a similar equation may be derived for the lateral flux.

From the continuity and vertical moisture flux equation, the time variation of soil moisture content for layer j is discretized as

$$\theta_j^{n+1} = \theta_j^n + (Q_{V_{j-1}} - Q_{V_j})(\Delta t/\Delta z), \tag{7}$$

where j is the space discretization, n is the time step, Δt is the time step size, and Δz is the layer thickness.

To apply (7) to boundary elements, information about the soil moisture flux across the boundary is required. For the lower boundary, (i) $Q_{V_N} = 0$ for a zero-flux boundary condition condition, (ii) $Q_{V_N} = K_N$ for a gravity-drainage boundary condition, or (iii) Q_{V_N} is estimated from (6a) using an imaginary soil layer below the bottom soil layer with zero thickness and fixed soil moisture content equal to the porosity of the bottom soil layer for a fixed water table at the base of the soil column. For the upper boundary, (i) Q_{V_1} may be specified as the actual evapotranspiration rate or estimated from the soil moisture content and potential evapotranspiration rate using a soil moisture stress index if there is an exfiltration event, or (ii) Q_{V_1} is estimated from (6a) using an imaginary soil layer above the soil surface of zero thickness and soil moisture equal to the porosity of the near-surface soil layer if there is an infiltration event with ponding.

d. Application to the Kalman filter

The Kalman filter assimilation scheme requires the soil moisture profile forecasting equation be in an explicit time-stepping form for forecasting of the covariances. However, explicit models can only take small time steps and hence run much more slowly than implicit models. On the other hand, nonlinear implicit models typically involve iteration until convergence at each time step. Because computation time was a major limitation with the one-dimensional synthetic study of Walker et al. (2001), a variation of the implicit scheme was used. If we write (7) in terms of the Crank–Nicholson implicit scheme (Gerald and Wheatley 1989), then

$$\theta_j^{n+1} - \frac{1}{2}\left[(Q_{V_{j-1}} - Q_{V_j})\frac{\Delta t}{\Delta z}\right]^{n+1} = \theta_j^n + \frac{1}{2}\left[(Q_{V_{j-1}} - Q_{V_j})\frac{\Delta t}{\Delta z}\right]^n. \tag{8}$$

Substituting for Q_V from (6) and assembling the global soil moisture state equation we can obtain an equation of the form

$$\mathbf{\Phi}_1^{n+1}\hat{\mathbf{X}}^{n+1/n} + \mathbf{\Omega}_1^{n+1} = \mathbf{\Phi}_2^n\hat{\mathbf{X}}^{n/n} + \mathbf{\Omega}_2^n, \tag{9}$$

where $\mathbf{\Phi}$ is the matrix of coefficients for the vector of moisture values $\mathbf{X}$, and $\mathbf{\Omega}$ is the vector of nonmoisture-dependent terms. The notation $n + 1/n$ is used to identify a forecast at time step $n + 1$ given the forecast at time step n.

After some algebraic manipulation of (9) we can obtain an explicit linear state space equation form, as required by the Kalman filter:

$$\hat{\mathbf{X}}^{n+1/n} = \mathbf{A}^n\hat{\mathbf{X}}^{n/n} + \mathbf{U}^n, \tag{10}$$

where

$$\mathbf{A}^n = (\Phi_1^{n+1})^{-1}(\Phi_2^n), \quad \text{and} \tag{11a}$$

$$\mathbf{U}^n = (\mathbf{\Phi}_1^{n+1})^{-1}(\mathbf{\Omega}_2^n - \mathbf{\Omega}_1^{n+1}). \tag{11b}$$

Once convergence of (8) has been achieved, the system state covariances may be forecast using the converged value for $\mathbf{A}$ from (11a). Using this approach, iteration is performed only for forecasting of the system states, with evaluation of $\mathbf{A}$ and forecasting of the system state covariances performed only once (after convergence of the system states), using a single large time step. Because forecasting of the system state covariance matrix is computationally the most demanding step of the Kalman filter, this implicit approach minimizes the computational effort required to forecast the system state covariances by the Kalman filter [for the Kalman filter equations see Walker et al. (2001)].

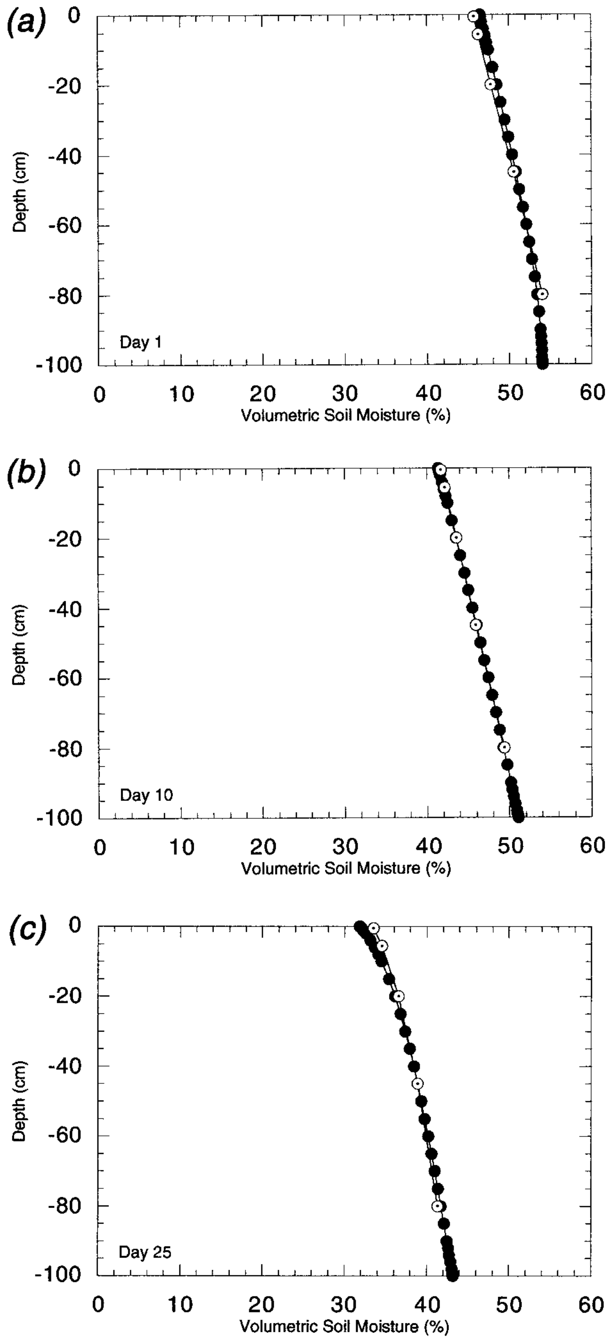


FIG. 2. Comparison of simulated soil moisture profiles using ABDOMEN for 5 soil layers (open symbols) and the Richards equation with 30 soil layers (closed symbols) for evaporation of 5 mm day^{-1}. Soil moisture with depth for times after the beginning of simulation: (a) 1, (b) 10, and (c) 25 days.

e. Model evaluation

To give credibility to the model and to verify the proposed form of the conceptual distribution factor, a comparison was made with the one-dimensional Richards equation. The simulation was for a 1-m soil column with the typical soil properties in Table 2. Two scenarios

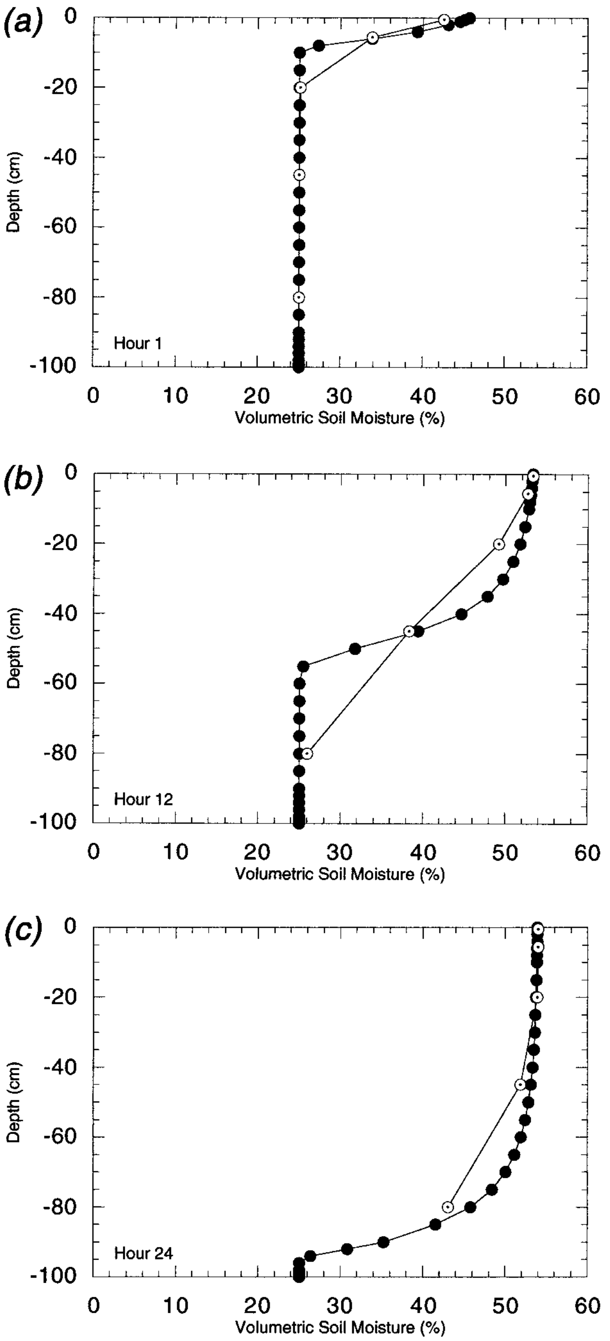


FIG. 3. Comparison of simulated soil moisture profiles using ABDOMEN for 5 soil layers (open symbols) and the Richards equation with 30 soil layers (closed symbols) for precipitation of 10 mm hr^{-1}. Soil moisture with depth for times after the beginning of simulation: (a) 1, (b) 12, and (c) 24 h.

were evaluated: (i) an exfiltration event of 5 mm day^{-1}, starting from an initially uniform soil moisture profile of 51.5% v/v (−500-mm matric head) and (ii) an infiltration event of 10 mm h^{-1} precipitation, starting from a uniform initial condition of 25% v/v (−13 620-mm matric head). Zero moisture flux was imposed at the base of the soil column for both scenarios.

The MGRAD parameter was evaluated from calibrating the ABDOMEN model with 30 soil layers to the exfiltration simulation using the Richards equation, with the ''NLFIT'' Bayesian nonlinear regression program (MGRAD = 280 mm). The NLFIT program suite (Kuczera 1994) is an interactive optimization package, employing the Shuffled Complex Evolution Method developed at The University of Arizona of Duan et al. (1994).

With the fitted MGRAD, the ABDOMEN model was run with five soil layers for the same exfiltration event used for calibration and for the independent infiltration event. The results from these simulations are given in Figs. 2 and 3, in which there is an extremely good agreement for all simulation times, particularly when taking into account layer thickness and that soil moisture content estimates are averages over the soil layer.

The above simulations showed that the ABDOMEN model is an excellent approximation to the Richards equation, even with only a few soil layers. To verify that ABDOMEN is appropriate for the Kalman filter assimilation scheme, the synthetic assimilation study of Walker et al. (2001) was repeated for an observation depth of 1 cm and observation frequency of once every 5 days, with the soil properties given in Table 2. In the study of Walker et al. (2001), a time series of ''true'' soil moisture profiles was generated with the Richards equation for a drying event. The simulation was then repeated with the same soil parameters and forcing data but poor initial conditions. Near-surface soil moisture data from the ''truth'' simulation were then assimilated with the Kalman filter for various observation depths and frequencies. This verification study uses the same forcing data, soil parameters, and initial conditions as the previous study.

Starting from a poor initial guess of 35.5% v/v (−3000-mm matric head), ABDOMEN was subjected to a constant evaporation rate of 5 mm day^{-1} and zero moisture flux at the column base. The model prediction was then updated with ''observations'' of the true soil moisture content in the top 1-cm layer. These observations were obtained from the true soil moisture profiles generated from the Richards equation model (i.e., initial condition of −500-mm matric head, Fig. 2). Figure 4 shows the results from assimilating near-surface soil moisture in the simplified model, in which the retrieved soil moisture profiles are compared with the open-loop simulation and the true soil moisture profiles from the Richards equation. The open-loop simulation is one in which no observations were used and the system was simply propagated from the initial conditions subject to the surface flux boundary conditions. The soil moisture profile for the poor initial condition is retrieved after 10 days (two updates).

The previous study by Walker et al. (2001) used a matric-head form of the Richards equation and found it

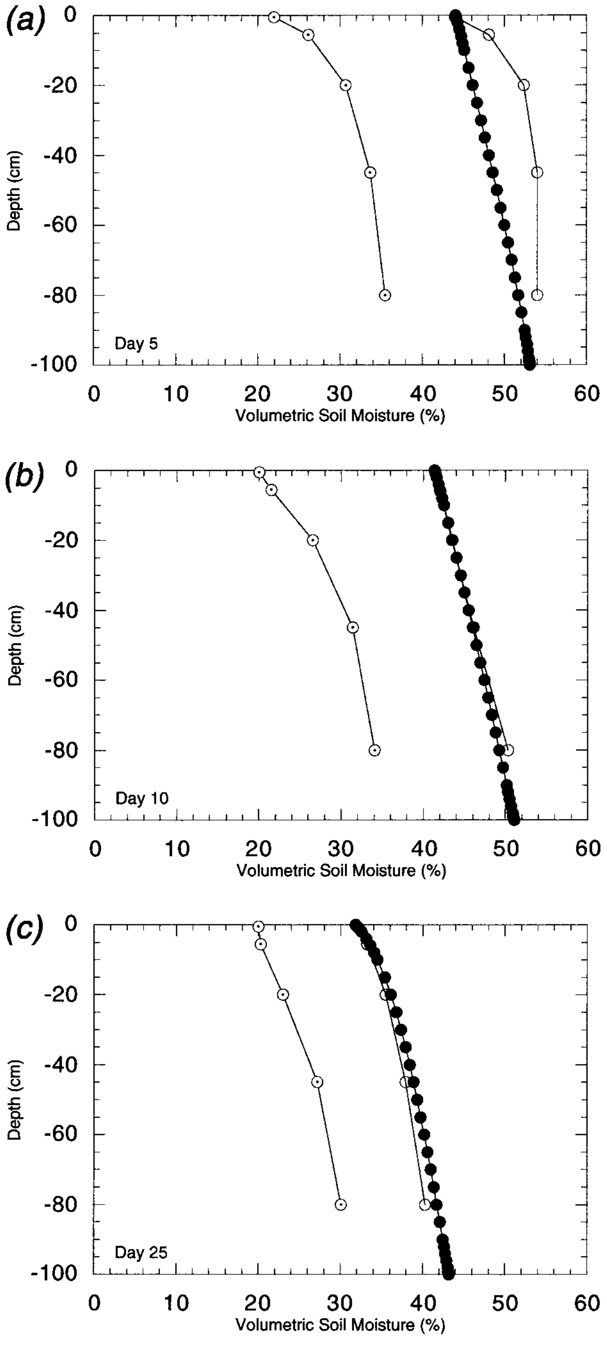


FIG. 4. Comparison of soil moisture profile retrieval using ABDOMEN (open symbol), the open-loop profile (open symbol with dot), and the Richards equation (closed symbol). The 5-layer model was updated once every 5 days using an observation depth of a 1-cm layer; initial variances were 0.25, system noise was 5% of the state per hour, and observation noise was 2% of the state. Soil moisture with depth for times after the beginning of simulation: (a) 5, (b) 10, and (c) 25 days.

TABLE 4. Model and measurement depths used in comparisons.

Model		Connector TDR		Virrib	
Layers	Depth (mm)	Probe length(s) (mm)	Depth (mm)	Sensors	Depth (mm)
1–3	0–123	100/150	0–125	1	0–160
1–4	0–235	200/300	0–250	1/2/3	0–260
1–5	0–460	400	0–400	1/2/3/4/5	0–460

necessary to apply a volumetric soil moisture transformation to the matric-head forecasts before assimilating near-surface soil moisture observations under these conditions, so as to avoid spurious updates. The results shown here confirm their recommendation—that a soil moisture–based model would alleviate the problems encountered with the more nonlinear matric-head model—and indicate that the ABDOMEN model is appropriate for assimilation of near-surface soil moisture data using the Kalman filter.

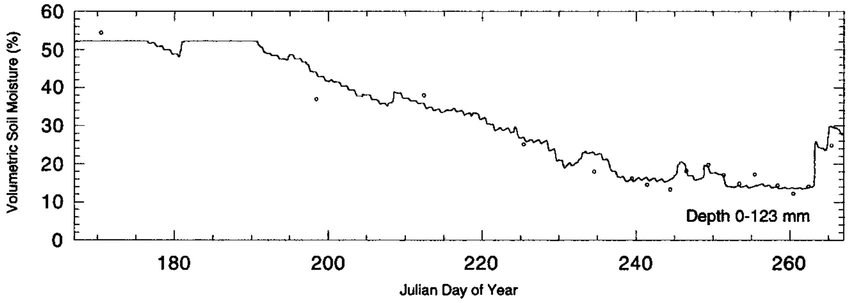
3. Field data

The field data used in this study are from the Nerrigundah experimental catchment (Walker 1999), located in a temperate region of eastern Australia. The main objective of this experimental catchment was to enable a soil moisture assimilation study at the catchment scale, which is to be the topic of a future paper. However, it also provided an excellent dataset for a field evaluation of soil moisture assimilation in a one-dimensional soil column, which is the topic of this paper. Only the data pertinent to this study are discussed here.

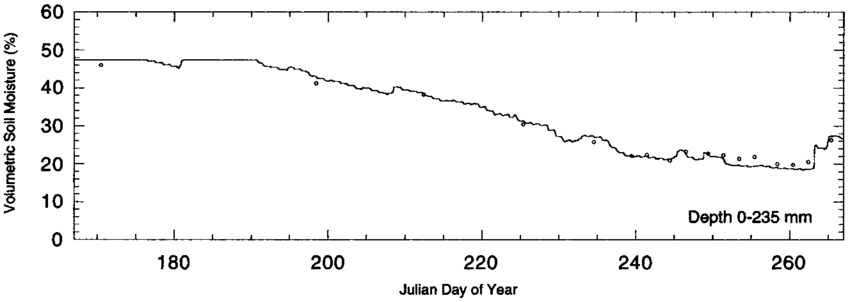
a. Monitoring and instrumentation

The Nerrigundah experimental catchment was instrumented from 12 October 1996 to 20 October 1998 for profiles of soil moisture content, soil temperature, and surface heat and soil moisture fluxes. The permanent instrumentation was located in a level area in the upper reaches of the catchment. Hence, the lateral redistribution of soil moisture should be negligible, making the data suitable for this study.

Permanent instrumentation in the Nerrigundah catchment consisted of a Campbell Scientific, Inc., automatic weather station (the mention of trade and company names is for the benefit of the reader and does not imply an endorsement of the product), which monitored (but was not limited to) relative humidity, air temperature, atmospheric pressure, precipitation, net radiation, soil heat flux, and wind speed. Apart from rainfall, all measurements were made at 1-min intervals, and the average was logged every 10 min. In addition to a collecting rain gauge, rainfall was recorded for each tip of the 0.2-mm tipping bucket. The weather station was located on a duplex soil with total depth of 46 cm. The soil moisture profile was continuously monitored using five ‘‘Virrib’’



(a)



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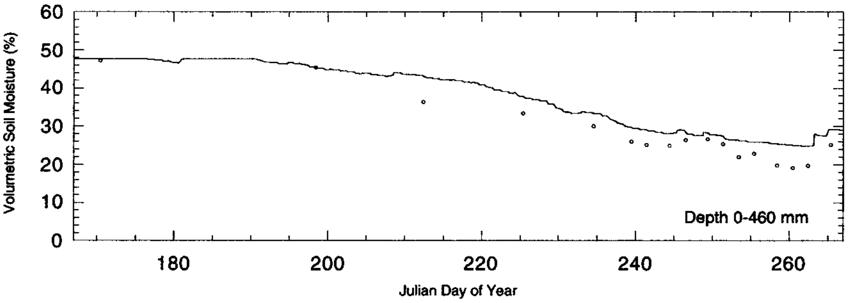


(c)

FIG. 5. Calibration of ABDOMEN (solid line) to connector TDR soil moisture measurements (open circles) from 16 Jun to 24 Sep 1997. The figure shows average soil moisture content over layers (a) 1–3, (b) 1–4, and (c) 1–5.

soil moisture sensors installed horizontally at depths of 10, 15, 20, 30, and 40 cm, providing soil moisture measurements over a layer thickness of 12 cm (according to Komin Technical Data, Inc.), and logged every 15 min. The minimum depth at which the Virrib sensor could be installed without having interference from the air layer above was 10 cm (according to Komin Technical Data).

In addition to the Virrib sensors, soil moisture measurements were made in the same location on a fortnightly basis, using vertically inserted connector time domain reflectometry (TDR) probes. The connector TDR probes gave an average soil moisture measurement over depths of 0–5, 0–10, 0–15, 0–20, 0–30, and 0–40 cm, the latter being the length of the probe. The TDR system used was the Soil Moisture Equipment Corporation (1989) TRASE TDR, using the standard TRASE calibration to determine the volumetric soil moisture content from the measured dielectric constant. The vertically inserted connector TDR probes were installed on 24 April 1997.

b. Soil moisture considerations

Comparison of connector TDR data with thermogravimetric measurements showed that the standard calibration was adequate for the 10-cm (standard deviation 2.8% v/v) and 15-cm (standard deviation 2.2% v/v) probe lengths, but the 5-cm (standard deviation 6.9%

v/v) probe lengths yielded a noisy response (Walker 1999). The calibration of longer TDR probes was not evaluated, because of the destructive nature and labor intensiveness of the testing, the number of calibration data values required to make conclusive statements regarding accuracy, and the good agreement for the shorter probes. In addition, literature suggests that longer probes should not result in loss of accuracy. An in situ calibration of the soil moisture sensors installed at the weather station could not be performed without destroying the soil moisture monitoring site. Hence, evaluation of soil moisture measurements was performed by making comparisons between the different soil moisture sensor types and using the calibration of connector TDR probes to give confidence in the connector TDR soil moisture measurements.

c. *Soil characterization*

The Nerrigundah soil was characterized by a combination of field and laboratory tests. Field tests included Guelph permeameter and double-ring infiltrometer tests for saturated hydraulic conductivity; laboratory tests on minimally disturbed soil cores included the determination of soil depth, soil horizons, soil bulk density and porosity, and particle size analysis. The results from these tests were available for locations within 2 m of the soil moisture monitoring site.

d. *Evapotranspiration*

Actual evapotranspiration was estimated from Penman–Monteith potential evapotranspiration and a soil moisture stress index. The soil moisture stress index is used to limit the potential evapotranspiration rate as a function of the available water in the soil. The soil moisture stress index used in this study was the average column soil moisture content divided by the average column porosity. Measurements of actual evapotranspiration using the eddy correlation technique on 6 days were used to verify the linear soil stress index used, with a correlation coefficient of 0.9.

4. Field application

In this section, the ABDOMEN model is calibrated and evaluated against the soil moisture profile measurements made in the Nerrigundah catchment. The calibrated model is then used for retrieval of the soil moisture profile by assimilation of near-surface soil moisture measurements.

a. *Calibration*

Soil moisture profile data from the connector TDR soil moisture sensors were used for calibration of ABDOMEN. Virrib data were not used for the final calibration, because much soil disturbance was required for their installation. Moreover, there were periods when Virrib data were inconsistent with rainfall measurements. Such inconsistencies were not found with the connector TDR data.

Because there were missing meteorological data between 24 and 27 September 1997, the model calibration was undertaken for soil moisture data collected prior to 24 September 1997, and model evaluation was done against soil moisture data collected subsequent to 27 September 1997. The calibration was performed on the 100-day drydown period from 16 June to 24 September 1997.

1) Observed model parameters

Several of the model parameters could be defined directly from field observations and measurements. Apart from layer 1 in the soil moisture model, soil layer thicknesses were set to the observed soil horizon thicknesses. Layer 1 was set at a thickness of 1 cm to be commensurate with the typical near-surface soil moisture observation depth from remote sensing at C band. The depression storage parameter was set at 5 mm, based on measurements of rms surface roughness made near the weather station. Likewise, the saturated hydraulic conductivity was estimated from the Guelph permeameter and double-ring infiltrometer measurements made near the weather station (Table 3). The porosity and residual soil moisture content for each of the model layers was estimated from an analysis of both Virrib and connector TDR soil moisture measurements made from 10 May 1997 to 1 October 1998. The soil porosity values were estimated as the maximum soil moisture content for the soil layer during periods of saturation and the residual soil moisture values were estimated as the minimum soil moisture content for the soil layer from periods when the soil was at its driest (during the summer of 1997/98).

2) Calibrated model parameters

After defining the above model parameters from field measurements and observations, the only parameters requiring calibration in the soil moisture model were the van Genuchten parameter n, relating hydraulic conductivity to saturated hydraulic conductivity, and MGRAD. Calibration of these parameters was performed with the connector TDR soil moisture measurements of depth-integrated soil moisture over model layers 1–3, 1–4, and 1–5 (see Table 4 for depth comparisons) with NLFIT.

Initial soil moisture values were set to the soil porosity values, given that calibration commenced when the soil was saturated. With the soil column being underlain by a layer of low-permeability sandstone, a zero-moisture flux boundary condition was applied to the base of the soil column. The surface soil moisture flux boundary condition was set at a fixed value for 0.5-h

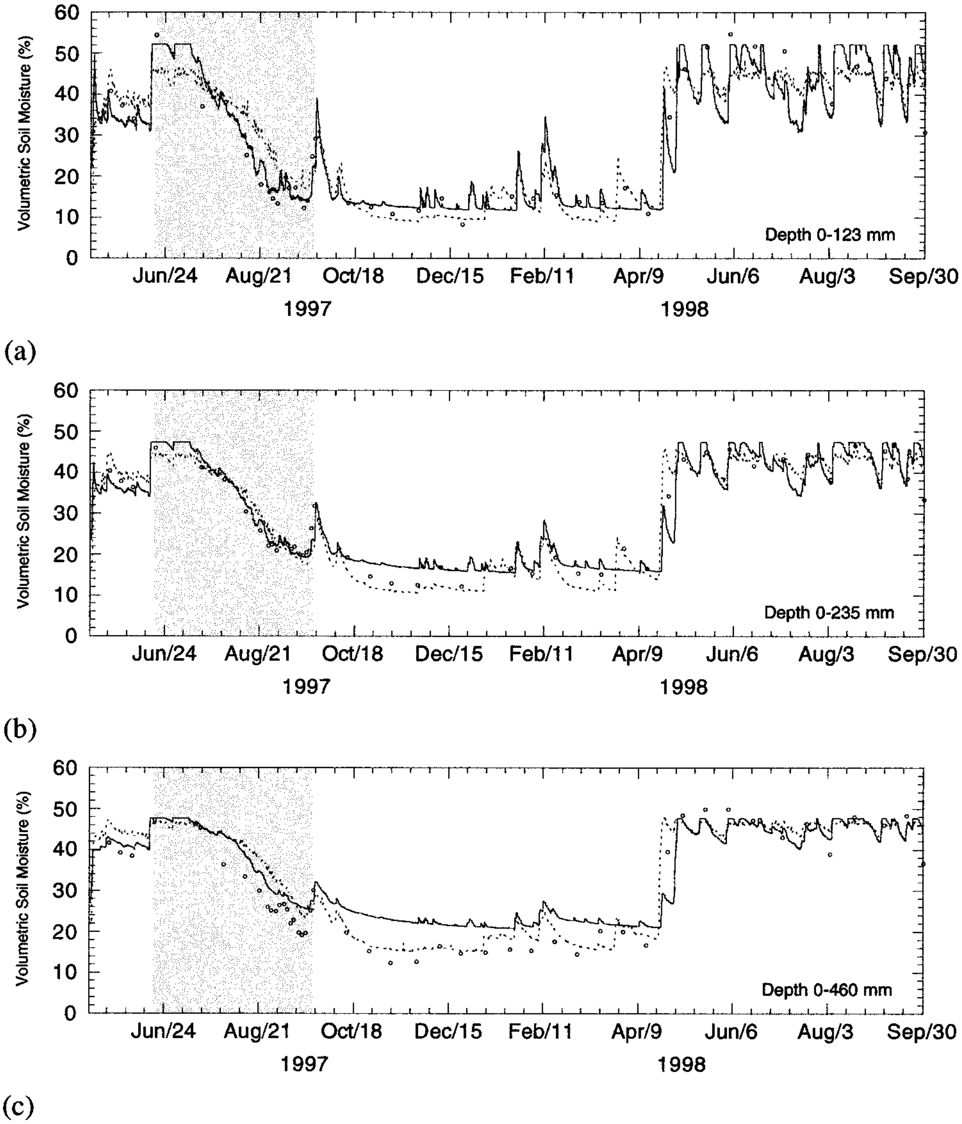
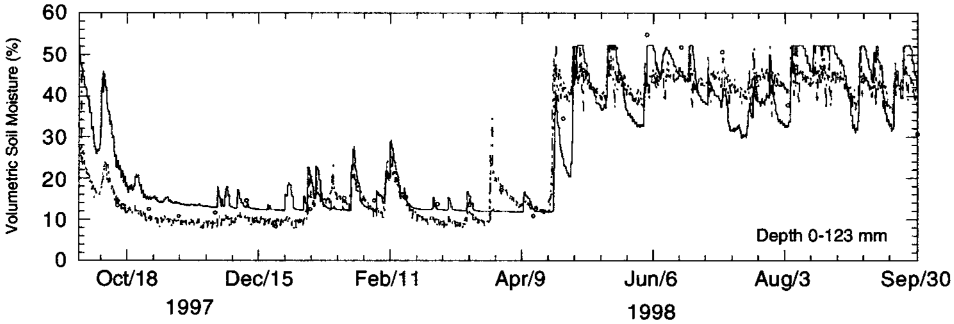


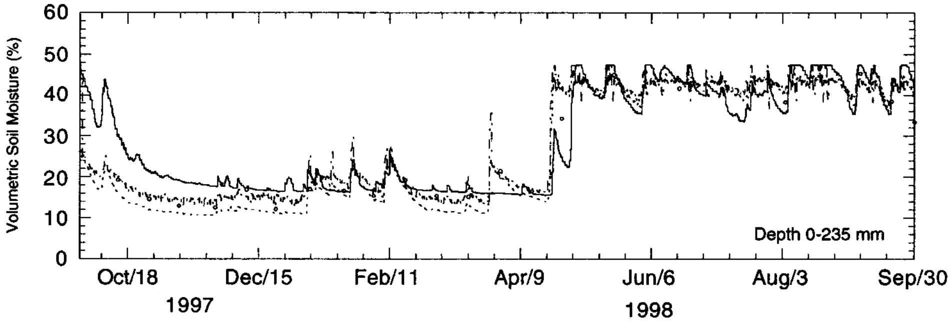
FIG. 6. Evaluation of ABDOMEN (solid line) calibration from 10 May 1997 to 1 Oct 1998 against Virrib (dashed line) and connector TDR (open circles) soil moisture measurements. The shaded region indicates the period of calibration with connector TDR soil moisture measurements. The figure shows average soil moisture content over layers (a) 1–3, (b) 1–4, and (c) 1–5.

simulation periods. This surface soil moisture flux was taken as the average of 10-min measurements of Penman–Monteith potential evapotranspiration rate, reduced by the soil stress index, except for periods during which there was rainfall recorded. During these periods, it was assumed that no evapotranspiration occurred and that the rainfall recorded had a uniform rainfall rate over the 0.5-h period. Ponding greater than the depression storage depth instantly went as runoff.

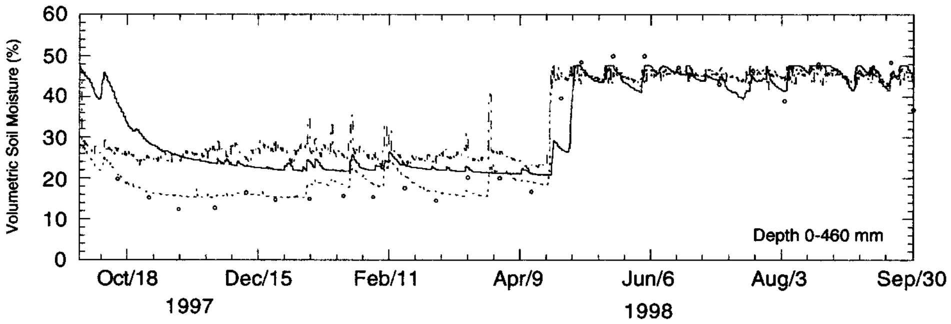
Parameters from calibration to the connector TDR data are given in Table 3, and the simulation results are compared with the connector TDR observations in Fig. 5. This and the following figures show depth-integrated soil moisture comparisons, because these were the data available from connector TDR measurements. Connector TDR data could not be converted readily to a soil layer measurement reliably, but Virrib and model output data could be easily converted to a depth-integrated value. These calibrated parameter values gave very good agreement with the connector TDR soil moisture data for model layers 1–3 and 1–4 but slightly overestimated the total column soil moisture. The consistent slight overestimation of soil moisture storage for the entire soil profile as compared with the connector TDR measurements may be a result of (i) the no-drainage boundary condition at the bottom of the soil profile, (ii) an incorrect estimate of rainfall and/or evapotranspiration, (iii) a systematic error in the model physics, or (iv) a



(a)



(b)



(c)

FIG. 7. Comparison of the retrieved soil moisture profile (dash–dot line) from updating with Virrib No. 1 soil moisture measurements in the top 123-mm soil layer with Virrib (dotted line) and connector TDR (open circle) soil moisture measurements and the open-loop simulation (solid line). The simulations were initiated with a poor initial guess of the soil moisture profile, that being the soil porosity; the soil moisture profile was updated once per day. The figure shows average soil moisture content over layers (a) 1–3, (b) 1–4, and (c) 1–5.

systematic error in the 40-cm TDR measurement. These factors are discussed further in the following section.

Calibration to Virrib data or Virrib and TDR data together was unable to improve the calibration. Moreover, the MGRAD values obtained from calibration to the connector TDR data increased with depth, which is consistent with the duplex soil characteristics observed; the clay content in the soil profile increased with depth so that the matric suction should be greater at deeper depths.

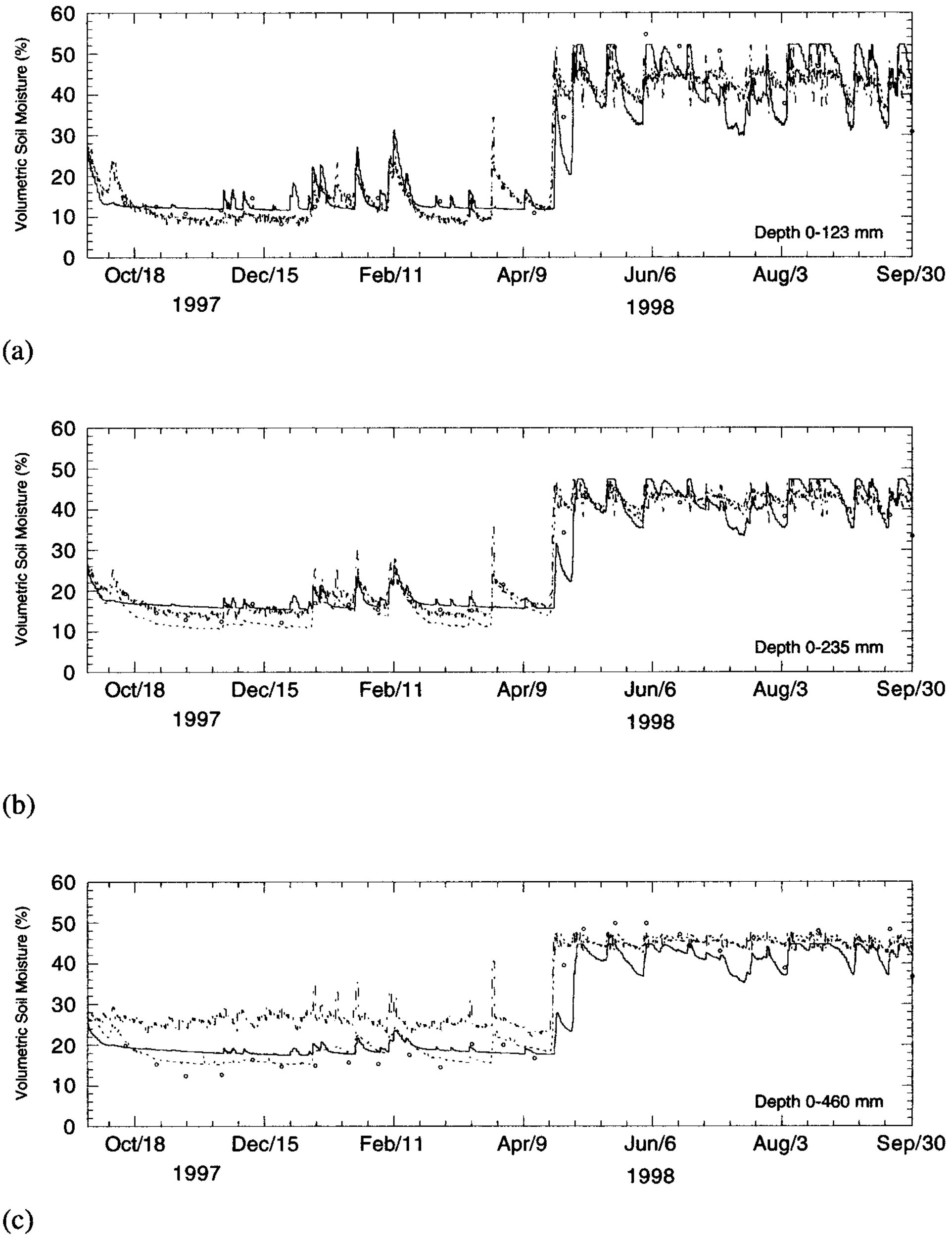


FIG. 8. Same as Fig. 7, but the simulations were initiated with a uniform soil moisture profile of 26.6% v/v from the near-surface soil moisture measurement.

3) EVALUATION

Using the calibrated parameters (Table 3), the soil moisture model was evaluated for the period from 10 May 1997 to 1 October 1998 using both the connector TDR and Virrib data. This dataset is independent of the calibration data. The simulation results from this evaluation are given in Fig. 6, in which there is good agreement with observed soil moisture data for the top 123 mm for the entire simulation period. The comparison with observed soil moisture data for the top 235 mm is also good, apart from a slight overestimation (5% v/v) of soil moisture content during the summer period. This overestimation of soil moisture during the summer period is greatest for the comparison with total profile soil moisture storage, with a maximum overestimation of about 10% v/v. This is consistent with the calibration results, for which the total soil moisture storage is overestimated by approximately 5% v/v.

Possible explanations for this overestimation are unaccounted-for gravity drainage and lateral redistribution. However, the effects of gravity drainage and lateral redistribution are greatest during periods of high soil moisture content, meaning that these factors may not explain the poor comparison during the summer months. Thus, we believe that the most likely reason for the poor comparison during dry periods is the estimation and/or application of evapotranspiration in the soil moisture model. In ABDOMEN, all evapotranspiration was subtracted directly from the near-surface soil layer. When the surface layer(s) approached the residual soil moisture content, the extraction of evapotranspiration was limited by the amount of available soil moisture in the surface layer and the rate of upward transport from deeper layers to provide water for evaporation from the surface layer. Hence, during the summer when near-surface soil moisture content approached the residual soil moisture content, evapotranspiration from the model profile would be less than it should be, resulting in an overestimation of the total soil moisture profile storage. One possible solution would be to include a root water uptake term in the soil moisture model, although that was not done here.

b. Soil moisture profile retrieval

The ability to retrieve accurately the soil moisture profile from near-surface soil moisture observations using the Kalman filter assimilation scheme under field conditions was evaluated from 27 September 1997 to 1 October 1998. In applying the Kalman filter, initial soil moisture states were given a standard deviation of 50% v/v and zero correlation between model layers for generating the initial system state covariance matrix, chosen to represent no prior knowledge of the soil moisture profile. The observation covariance matrix consisted of a single value, that being the variance of the near-surface soil moisture observation. A value of 2% of the observation was used as the standard deviation of observations, because this value was found to be the accuracy of the soil moisture measuring device. The system noise matrix was given a value of 5% of the system states per 0.5 h of simulation time for diagonal elements and zero for off-diagonal elements, because it ensured that model error was greater than observation error and was consistent with our belief in the accuracy of the model.

Data from the Virrib sensor in closest proximity to the soil surface were used as our observations of the near-surface soil moisture. These data were used in preference to the connector TDR data because they were monitored continuously, rather than only once every fortnight. This allowed for greater flexibility in testing different updating intervals used in simulations. The near-surface Virrib data were found to have good agreement with both the connector TDR data and model simulation (Fig. 6a). Because the Virrib measurements were being made in the 40–160-mm depth range, the soil moisture observations for data assimilation were applied over an observation depth of 123 mm (layers 1–3), that being the approximate depth of the near-surface soil moisture observations. In the assimilation, the Kalman filter observation equation compares the observed soil moisture in the top 123 mm of soil to the model soil moisture forecast in the top three layers and makes an adjustment to all five model layers through the correlation between the near-surface and deep soil layers in the forecast model covariance matrix. Although this depth of observation is not directly comparable with that applicable to current remote sensing, it is the shallowest depth of soil moisture measurement available from these field data. Moreover, it allows us to gain insight and to make important advances toward the use of actual remotely sensed near-surface soil moisture data in future studies.

1) Updating once every day

For the first run with the soil moisture profile retrieval algorithm using the Kalman filter assimilation scheme, the model was initialized with a poor initial soil moisture profile, representative of the situation in which one has no prior knowledge of the true soil moisture condition. The initial soil moisture values used were the porosity values of each model layer. The soil moisture forecasting model was then run, subject to the surface forcing data, and updated once every day with near-surface Virrib soil moisture measurements for the 123-mm depth. The results from this simulation are compared with the open-loop simulation (no updating of the soil moisture model), Virrib soil moisture data, and connector TDR soil moisture data in Fig. 7.

The results from this simulation show that the soil moisture profile retrieval algorithm using the Kalman filter assimilation scheme quickly brings the soil moisture model on track to a depth of 235 mm. The retrieval of soil moisture content in the top 123 mm of the profile follows the Virrib soil moisture measurements almost exactly, as expected, and retrieval of soil moisture content in the top 235 mm follows both the Virrib and connector TDR soil moisture measurements very closely. However, during the dry summer period, the estimated soil moisture content for the entire soil profile was greater than the measured soil moisture content. The reason for the forecasting model simulating the near-surface soil moisture content correctly yet overpredicting the total soil moisture storage is evident from Fig. 6. During the dry summer period, the model simulates the near-surface soil moisture content accurately but overestimates the total soil moisture profile storage. If this systematic error did not exist in the forecasting model, then the simulation of the soil moisture profile would have continued to track the measured soil moisture profile correctly once the measured soil moisture profile was retrieved. Hence, the Kalman filter retrieval of the soil moisture profile is only as good as the model prediction of the soil moisture profile for a given near-surface soil moisture content.

Although the retrieved column soil moisture was overpredicted in comparison with the observations, the

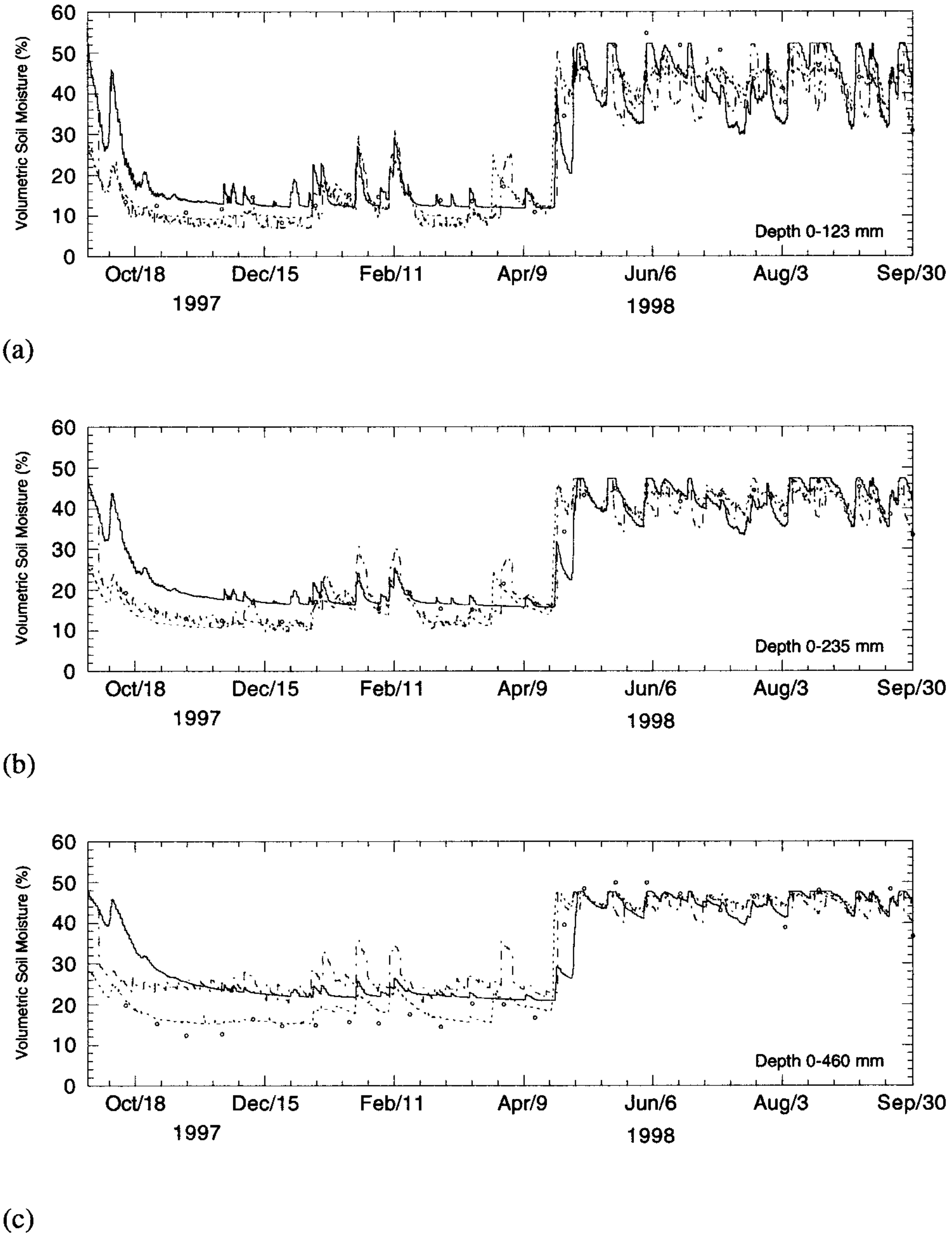


FIG. 9. Same as Fig. 7, but the soil moisture profile was updated once every 5 days.

retrieved soil moisture was generally an improvement on the open-loop simulation, particularly during the first four months. After this lead period, retrieved soil moisture to a depth of 235 mm continued to be an improvement on the open loop, and the open loop was a slight improvement on the retrieval for the total soil column.

Note also that the open-loop simulation started to follow the observed soil moisture closely toward the end of the dry summer period and continued to simulate the soil moisture profile storage correctly through the wet winter months. This result suggests that profile soil moisture may be simulated correctly during sustained dry periods and sustained wet periods, without assimilation of near-surface observations, providing the correct porosity and residual soil moisture values are given to the model. Thus, the forecasting model resets itself whenever it hits a state boundary (i.e., dry or saturated). However, during dynamic wetting/drying periods, assimilation of near-surface soil moisture observations is important for correct simulation of the soil moisture profile.

The sensitivity of profile retrieval to the initial soil moisture condition was assessed by initializing ABDOMEN with a soil moisture profile that was close to the correct value. In this simulation, the initial soil moisture profile was estimated by applying uniform soil

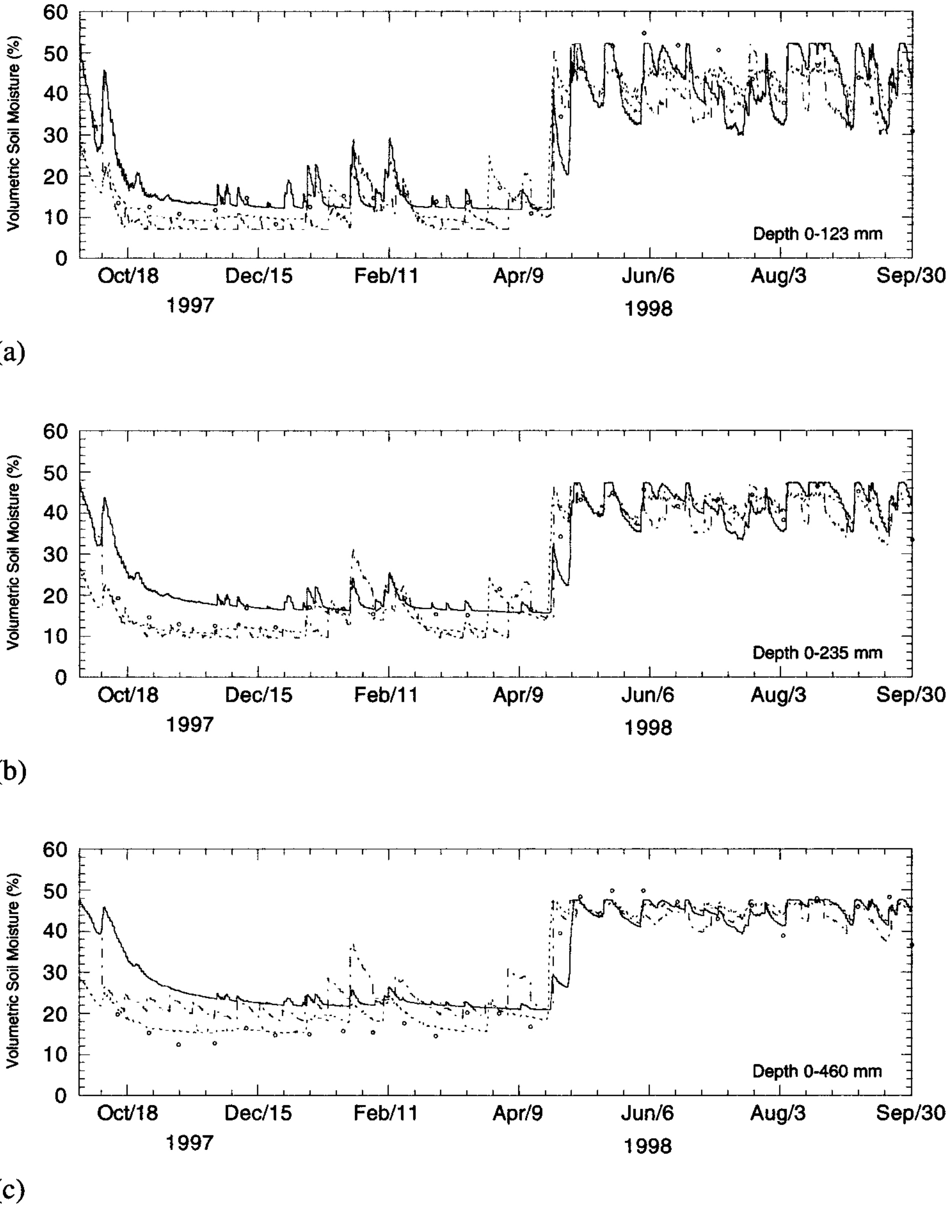


FIG. 10. Same as Fig. 7, but the soil moisture profile was updated once every 10 days.

moisture content throughout the profile, using the near-surface Virrib sensor measurement. The retrieval results from this simulation (Fig. 8) are identical to the retrieval results in Fig. 7. However, the open-loop simulation was able to track the observed soil moisture profile very closely in this simulation. This is because the initial soil moisture values were close to the correct values for near-surface layers and slightly less than the correct values for deeper layers. The effect of this was to offset the influence of no root water uptake seen in Fig. 6.

2) Updating at low temporal resolutions

Updating with near-surface soil moisture observations once per day may be feasible for some low-spatial-resolution satellites, such as current-generation passive microwave sensors, but updating with high-spatial-resolution observations, such as those from current-generation active microwave sensors, requires updating with a much lower temporal resolution. In addressing the effects from less frequent updating, simulations have been run with the forecasting model updated once every 5, 10, and 20 days. These simulation results are given in Figs. 9, 10, and 11, respectively, with the initial soil moisture profile set to the porosity.

The simulation results from less frequent updating suggest that total soil moisture profile storage is simulated more accurately as the update frequency is reduced, but the near-surface soil moisture is modeled

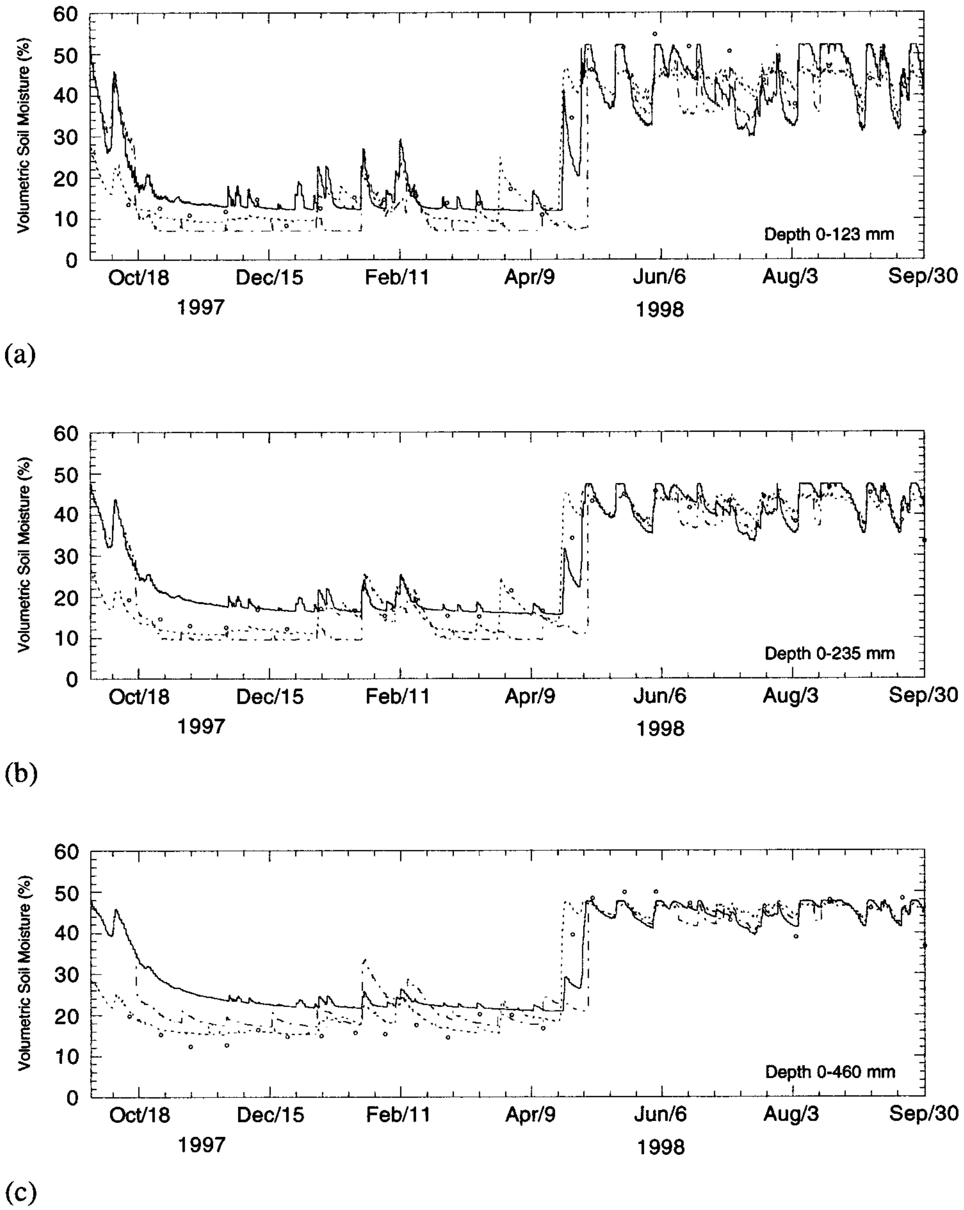


FIG. 11. Same as Fig. 7, but the soil moisture profile was updated once every 20 days.

more poorly. The reason is most evident from Fig. 11, in which it can be seen that the forecast near-surface soil moisture content was updated to the observed near-surface soil moisture content at each update step, with a corresponding increase in the soil moisture content of the deeper soil layers.

During the interobservation period, the forecasting model predicted a drydown of the entire soil profile, with near-surface soil moisture content estimates being less than the observed near-surface soil moisture content and the total soil moisture profile storage estimate approaching the observed total soil moisture profile storage. When the forecast model was updated more frequently, as in Figs. 9 and 10, the model was forced to follow the near-surface soil moisture content more closely. The effect of this forcing was a poorer retrieval of the total soil moisture storage. This was a result of the systematic error in the soil moisture forecasting model and insufficient time for the forecasting model dynamics to influence the soil moisture profile retrieval significantly.

The systematic error observed in the forecasting model was that, for a given near-surface soil moisture content greater than the residual soil moisture content, the model predicted a greater total soil moisture storage than that observed in the field. This was also noted in Fig. 6 and is believed to result from the forecasting model not having a root water uptake term. By including a root water uptake term in the soil moisture model, a drier total soil moisture profile storage could be predicted for a given near-surface soil moisture content, meaning that the Kalman filter would be able to estimate better the soil moisture profile from observations of the near-surface soil moisture content. These simulations would suggest that retrieval of the correct soil moisture profile using the Kalman filter assimilation scheme is more dependent on the forecasting model being able to forecast adequately the soil moisture profile dynamics than on the frequency of updating information. It does not mean that infrequent updating is more desirable than frequent updating, just that it is important to have an unbiased forecast model in order to obtain an unbiased model update.

c. Discussion

This study has yielded several important insights that will require careful consideration in future assimilation studies at both the one- and three-dimensional levels. Most important, if either the model forecasts or observations are systematically biased in any way, then without the removal of such biases it will be impossible to improve the forecast of the soil moisture profile, no matter how good the assimilation scheme is. Although the effect of model bias on the assimilation is not directly obvious, it has serious implications for application to real-life situations. This means that assimilation of near-surface soil moisture observations for retrieval of the soil moisture profile is only useful when errors in the soil moisture forecasts derive directly from errors in the initial conditions and/or atmospheric forcing data and not as a result of error in the physics of the soil moisture model.

Model and observation bias are potentially serious, but there are other secondary factors, including the initial conditions, soil type, observation frequency, and model approximation. Of these factors, model approximation is potentially the most serious. However, providing the model approximation does not introduce a systematic bias in the model, such as neglect of the root water uptake, the use of approximations in the forecasting model probably has no detrimental effect on the assimilation. Soil porosity and residual soil moisture content are the most important soil parameters for correct retrieval of the soil moisture profile. A residual soil moisture content that is too high or a soil porosity value that is too low will restrain the forecasting model from ever reaching the correct soil moisture content during extreme wet or extreme dry periods, even with an assimilation scheme.

5. Conclusions

In this paper, a computationally efficient soil moisture model has been developed, based on a conceptualization of the Buckingham–Darcy moisture flux equation. Although the simplified soil moisture model was a good approximation to the Richards equation, even when using only a few soil layers, a root water uptake term should be added to simulate field-measured soil moisture accurately. Without the root water uptake term or calibration to extreme drying events, the model overpredicts the soil moisture of deeper soil layers during extreme drying events.

Simulation results have indicated that, providing the soil porosity and residual soil moisture content parameters have been identified correctly, the soil moisture profile may be modeled correctly during sustained dry and sustained wet periods without assimilation of near-surface soil moisture observations, meaning that the forecasting model resets itself whenever it hits a state boundary. However, during dynamic wetting and drying periods, assimilation of near-surface soil moisture observations is important for correct simulation of the soil moisture profile.

Our results indicate that soil moisture profile retrieval with the Kalman filter assimilation scheme is only as good as the model representation of the dominant soil physical processes and its calibration. When the model overpredicts or underpredicts the soil moisture profile for a given near-surface soil moisture content, then the retrieved soil moisture profile is likely to be poor. Moreover, retrieval of the soil moisture profile using the Kalman filter assimilation scheme has been shown to be more dependent on the adequacy of the forecasting model to predict correctly the soil moisture profile dynamics than on the temporal resolution of near-surface soil moisture measurements. This result means that assimilation of near-surface soil moisture observations is only useful for correcting error in soil moisture forecasts as a result of errors in initial conditions and/or atmospheric forcing data and not as a result of error in the physics of the soil moisture model.

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