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Robust simulation of root zone soil moisture with assimilation of surface soil moisture data

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Abstract. An operational framework is presented for assimilating surface soil moisture remote sensing measurements into a soil-vegetation-atmosphere-transfer (SVAT) model for the robust prediction of root zone moisture time series. The proposed approach is based on analytical treatment of the dynamical equations coupling surface and deeper soil reservoirs. The resulting framework uses biases between observed and modeled time rates of change of surface soil moisture to quantify biases between modeled and actual root zone average soil moisture contents. The approach is based on the popular interactions between soil-biosphere-atmosphere (ISBA) force-restore SVAT model. An experimental data set, collected near Cork, Ireland, is analyzed both for a long data series of 183 days and four short periods that were selected to focus on different hydrometeorological conditions. The results demonstrated that the proposed framework performs uniformly robust over 3 orders of magnitude of misspecification of saturated hydraulic conductivity. In the presence of uncertain initial conditions, the results demonstrated a marked increase in model skill (over the original ISBA model) for periods when average precipitation was less than average potential evaporation.

1. Introduction

The exchange of heat and moisture between the land surface and the atmosphere drives weather and climate systems. The states of the surface and root zone soil moisture reservoirs are key variables controlling surface water and energy balances. Consequently, there is a need for accurate spatial and temporal representation of soil moisture in models of hydrologic (flood forecasting, irrigation, and agriculture) and atmospheric processes. Soil-vegetation-atmosphere-transfer (SVAT) models have been developed to simulate these mass and energy transfers and to update the soil moisture and thermal conditions through time from the solution of surface moisture and energy balance equations [e.g., *Noilhan and Planton*, 1989; *Famiglietti and Wood*, 1994; *Wigmosta et al*., 1994].

The accuracy of the land surface flux estimates is often limited by the accuracy of the soil moisture predictions [*Koster and Milly*, 1997]. Soil moisture model skill is typically limited by a combination of uncertainty in the initial conditions of the state variables and uncertainty in model physical and biological parameters. These problems are even more pronounced when attempting to model a large spatial domain. To compensate for these uncertainties, there has been a heightened effort at data assimilation, seeking to guide models with periodic observations of certain state variables, such as surface soil moisture. This merger of measurements and models through data assimilation is intended to provide optimal estimates of the state of the natural environment in the face of uncertain initial conditions and incomplete knowledge of soil and vegetation properties. Since the models are applied to provide spatially distributed predictions, the data sets used in the assimilation should have similar geographic coverage. The only general hope of obtaining such distributed observations of large-scale spatial fields of land surface variables is from remote measurement platforms [*McLaughlin*, 1995].

Ottlé and Vidal-Madjar [1994] used visible and thermal infrared remotely sensed data to constrain the surface soil moisture simulated by a catchment scale hydrological model, with a surface energy balance providing the link between moisture status and the radiative brightness temperature of the surface. While these preliminary results are encouraging for remote sensing applications, the comparison with data suggests significant room for improvement. *Houser et al*. [1998] updated surface soil moisture state observations in the three-layer topographically based land-atmosphere transfer scheme (TOPLATS) model [*Famiglietti and Wood*, 1994] through a range of techniques with mixed results regarding the root zone. They concluded that assimilation methods of moderate complexity are preferable to more complex techniques.

While passive and active microwave sensors have been useful for estimating spatial fields of soil moisture [*Jackson*, 1997; *Giacomelli et al*., 1995; *Altese et al*., 1996; *Bolognani et al*., 1996; *Mancini et al*., 1999], these measurements typically probe only the thin surface soil layer (5–10 cm). However, hydrologic and

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meteorological models require information about the soil moisture content in the full root zone. The possibility of estimating the root zone soil moisture from knowledge of the surface soil moisture status has been addressed by several authors, with approaches ranging from an empirical linear regression [*Arya et al*., 1983] to knowledge-based approaches that use a priori information about the soil hydrologic properties and assumptions regarding the hydrodynamic status [*Jackson*, 1980; *Camillo and Schmugge*, 1983; *Newton et al*., 1983]. *Jackson* [1980] demonstrated that the soil moisture profile can be estimated reasonably with an assumption of vertical hydraulic equilibrium (i.e., hydrostatic) on a daily time step. *Camillo and Schmugge* [1983] retrieved root zone soil moisture estimates from surface measurements for dry soils with fully grown roots using a linear relationship between moisture contents in the two soil layers based on a simple solution of Richards equation.

More recently, *Entekhabi et al*. [1994] demonstrated a solution of the inverse problem for the retrieval of soil moisture and temperature profiles from remotely sensed observations of multispectral irradiance using the extended Kalman filter. The Kalman filtering algorithm, which is based on the linearization of the state and measurement equations, is widely used for data assimilation in meteorology and hydrology because it permits a rigorous treatment of the fundamental sources of uncertainty from measurement error, model error and parameter variability [*McLaughlin*, 1995]. *Galantowicz et al*. [1999] tested the one-dimensional (1-D) assimilation methodology introduced by *Entekhabi et al*. [1994] to retrieve the soil moisture profile from periodic radiobrightness data for an 8 day field experiment and a 4 month synthetic study. *Walker et al*. [2001] used a Kalman filter-based assimilation to retrieve (estimate) the soil moisture profile directly from synthetic surface soil moisture observations. Assimilation of active microwave observation data into a model of the unsaturated zone for estimation of the soil moisture profile status for bare soils was recently conducted by *Hoeben and Troch* [2000], using the extended Kalman filter and a one-dimensional implementation of Richards equation. *Hoeben and Troch* [2000] reported excellent performance in the presence of known soil hydraulic properties and a high-resolution implementation of Richards equation for frequency of assimilation of at least 1 day^{-1}.

From an operational point of view, there remains a need for a robust integration of periodic surface remote sensing information into a dynamic soil water balance model to improve the simulation of root zone soil moisture [*Ragab*, 1995]. Moreover, there is need for a system that is both applicable over a wide range of conditions, where the vertical profile may not be hydrostatic, and computationally simple for application over large distributed domains. The availability of high-quality remote sensing data will often be limited to a daily frequency, while a dynamic SVAT model typically runs at temporal resolutions of 1 hour or finer. SVAT models typically include a thin surface soil layer and one or more thicker layers comprising the remainder of the root zone. The surface layer is the region that may be observed, or partially observed, by remote microwave sensors. However, this represents a small part of the entire root zone. Attempts are now focusing on assimilating surface remote sensing observations to improve predictions in the entire root zone. For the two soil compartment (thin surface layer and total root zone) SVAT models (e.g., interactions between soil-biosphere-atmosphere (ISBA) model of *Noilhan and Planton* [1989]) a vertical Kalman filter algorithm does not seem appropriate. The filter is more attractive for fine-resolution profiles, where error-covariance matrices are most appropriate and useful [*Walker et al*., 2001].

Approaches that update only the state of the observed layer typically do not improve model skill in the bulk of the root zone [*Li and Islam*, 1999]. Consequently, it seems reasonable to conclude that an operational assimilation of remotely sensed near-surface data into a SVAT model must include the ability to update the root zone status as well as the surface status. *Wigneron et al*. [1999] used the ISBA model and the results of *Mahfouf* [1991] and *Calvet et al*. [1998] in a study using the surface moisture estimates to retrieve the initial value of the root zone soil moisture for two long data sets over soybean crops. This retrieval algorithm estimates the initial conditions of the root zone soil water content by minimizing the root-mean-square error (RMSE) between daily measured and simulated surface soil moisture. *Wigneron et al*. [1999] highlighted the necessity for an integration period of at least 20–30 days for acceptable estimation of the initial root zone status. The approach performed well; however, the "hindcasting" nature of the statistical inversion is not particularly well suited for an operational system.

In this paper we derive and apply an operational assimilation protocol that incorporates periodic surface moisture observations to dynamically constrain the root zone soil moisture. We base the protocol development on the ISBA force-restore method [e.g., *Noilhan and Planton*, 1989; *Noilhan and Mahfouf*, 1996] with modifications developed for a stratified soil [*Montaldo and Albertson*, 2001]. We assess the predictive skill using a long time series of meteorological and soil moisture data available for a site in Cork, Ireland [*Albertson and Kiely*, 2001]. The in situ surface soil moisture observations are used as a proxy for the remote sensing information and measurements errors are not explicitly considered. We use the term "data assimilation" here in a broad sense, where data is assimilated (however crudely) into a model. Future work would be required to cast the work presented here in a more formal assimilation context, where measurement and model errors could be treated simultaneously and even optimally, such as with the extended Kalman filter.

2. Theoretical Development

In this section we describe briefly the SVAT model as modified to handle stratified soils, and we present the analytical basis for the assimilation of surface moisture observations into the root zone simulation.

2.1. Force-Restore SVAT Modeling Approach

The evolution of the surface thermal status is based on a "forcing" by the net energy exchange with the atmosphere (i.e., net radiation–sensible heat flux–latent heat flux) and a "restoring" action drawing the surface temperature toward the deep (or average) soil temperature [*Bhumralkar*, 1975; *Blackadar*, 1976; *Deardorff*, 1978]. The force-restore approach has been extended, by analogy, to simulate soil moisture content [*Deardorff*, 1978]. On the basis of its parsimonious parameterization and reasonable skill, this approach is widely used in practice [e.g., *Noilhan and Planton*, 1989; *Hu and Islam*, 1995; *Noilhan and Mahfouf*, 1996; *Lo Seen et al*., 1997; *Albertson and Kiely*, 2001] and, consequently, provides a sound and practical basis for the development of an operational assimilation protocol

[*Mahfouf*, 1991; *Calvet et al*., 1998; *Wigneron et al*., 1999; *Ragab*, 1995; *Li and Islam*, 1999].

We start with the ISBA force-restore model, which is well described elsewhere [*Noilhan and Planton*, 1989; *Noilhan and Mahfouf*, 1996]. For context, we present the soil moisture evolution equations here. The model considers the near-surface and total root zone soil layers of depths d_1 and d_2 and volumetric water contents θ_g and θ_2, respectively, which evolve according to

$$\frac{\partial \theta_g}{\partial t} = \frac{C_1}{\rho_w d_1}(P_g - E_g) - \frac{C_2}{\tau}(\theta_g - \theta_{\text{geq}}) \qquad 0 \le \theta_g \le \theta_s \quad (1)$$

$$\frac{\partial \theta_2}{\partial t} = \frac{1}{\rho_w d_2}(P_g - E_g - E_{tr} - q_2) \qquad 0 \le \theta_2 \le \theta_s, \quad (2)$$

where P_g is the precipitation infiltrating into the soil, E_g is the bare soil evaporation rate at the soil surface, E_{tr} is the transpiration rate from the root zone (d_2), q_2 is the rate of drainage out of the bottom of the root zone, ρ_w is the density of the water, θ_s is the saturated soil moisture content, C_1 and C_2 are the force and restore coefficients for soil moisture, and θ_{geq} is the equilibrium surface volumetric moisture content describing the hypothetical reference moisture value for which gravity balances the capillary forces such that there is no vertical water flow crossing the base of the thin surface layer of depth d_1 [*Noilhan and Planton*, 1989]. We adopt the unit gradient assumption of gravity drainage from the root zone, so that $q_2 = k_2$ (where k_2 is the hydraulic conductivity of the root zone at θ_2) [*Albertson and Kiely*, 2001]. The C_1, C_2, and θ_{geq} formulations are centrally important to the assimilation approach proposed here because they impact the evolution of θ_g, and it is our intent to make use of discrepancies between the tendency (i.e., time rate of change) of modeled and observed θ_g values to adjust the course of θ_2. For this reason, we review briefly the modification employed for the restoring term in (1) [*Montaldo and Albertson*, 2001].

The value of θ_{geq} was originally presented to be a function of θ_2 and the soil profile's hydraulic properties, derived from an approximate solution of Richards equation [*Noilhan and Planton*, 1989],

$$\theta_{\text{geq}} = \theta_2 - a\,\theta_s\left(\frac{\theta_2}{\theta_s}\right)^p\left[1 - \left(\frac{\theta_2}{\theta_s}\right)^{8p}\right], \quad (3)$$

with parameters a and p adjusted according to soil texture, accounting effectively for soil hydraulic properties. The relationships between soil moisture θ, hydraulic conductivity k, and matric potential ψ are described by

$$\psi = \psi_s\left(\frac{\theta}{\theta_s}\right)^{-b} \quad (4)$$

$$k = k_s\left(\frac{\theta}{\theta_s}\right)^{2b+3}, \quad (5)$$

where k_s is the saturated hydraulic conductivity, ψ_s is the air entry potential, and b is the slope of the retention curve in logarithmic space [*Clapp and Hornberger*, 1978]. Finally, the force and restore coefficients C_1 and C_2 are described by their original formulations:

$$C_1 = C_{1\text{sat}}\left(\frac{\theta_s}{\theta_g}\right)^{b/2+1} \quad (6)$$

$$C_2 = C_{2\text{ref}}\left(\frac{\theta_2}{\theta_s - \theta_2 + \theta_l}\right), \quad (7)$$

where $C_{1\text{sat}}$ and $C_{2\text{ref}}$ are parameters capturing effects of soil texture and θ_l is a small numerical value that constrains C_2 as θ_2 approaches θ_s [*Noilhan and Planton*, 1989].

In stratified soils, where the soil hydraulic properties and textural characteristics differ from the surface layer to the deep soil, (3) does not provide a reasonable approximation to the Richards equation [*Montaldo and Albertson*, 2001]. In fact, for certain soil profiles it is common to have upward soil water flux when the soil moisture decreases with depth (and vice versa) because of the different mapping by (4) along the vertical. *Montaldo and Albertson* [2001] developed and tested a simple approach for rescaling the root zone soil moisture to an "equivalent" root zone soil moisture that more accurately reflects (in evaluation against θ_g) the vertical water flow status for arbitrarily stratified soils. The rescaled root zone moisture status is given by

$$\hat{\theta}_2 = \theta_{s,g}\left(\frac{\theta_2}{\theta_{s,2}}\right)^{b_2/b_g}\left(\frac{\psi_{s,2}}{\psi_{s,g}}\right)^{-1/b_g}, \quad (8)$$

where the subscripts g and 2 indicate the soil parameters of the surface layer of depth d_1 and the total root zone of depth d_2, respectively. In this way, the values of $\hat{\theta}_{\text{geq}}$ from (3) and C_2 from (7) are calculated using $\hat{\theta}_2$, such that the restoring term of (1) more accurately reflects the drainage and recharge fluxes across the bottom of the surface layer $(z = d_1)$. For simplicity we drop the circumflex in the remainder of the paper. All the model runs in this paper employ this solution for stratified soils. We note, for context, that the SVAT model is integrated with a time step of Δt_1 (e.g., hourly), and we progress to introduce the assimilation of observations on a coarser time step Δt_2 (e.g., daily).

2.2. Data Assimilation

This section presents the analytical support for the proposed 1-D soil moisture assimilation protocol for updating both the near-surface moisture θ_g and the root zone soil moisture content θ_2 from θ_g observations in a manner that compensates for both inaccurate initial conditions and potential model bias resulting from imperfect model parameter estimates. The motivation is to improve on earlier efforts that either simply updated near-surface soil moisture without regard to θ_2 or updated θ_2 on the basis of a priori assumptions about the instantaneous relationship between θ_2 and θ_g.

We begin by writing the surface moisture balance once for model variables and separately for observed or actual variables. It is reasonable to expect (1) to be valid for each set of variables. Hence, indicating the model variables with the superscript m and the corresponding values that could be observed (i.e., actual) with the superscript o, we have

$$\frac{\partial \theta_g^m}{\partial t} = \frac{C_1^m}{\rho_w d_1}(P_g^m - E_g^m) - \frac{C_2^m}{\tau}(\theta_g^m - \theta_{\text{geq}}^m) \quad (9)$$

$$\frac{\partial \theta_g^o}{\partial t} = \frac{C_1^o}{\rho_w d_1}(P_g^o - E_g^o) - \frac{C_2^o}{\tau}(\theta_g^o - \theta_{\text{geq}}^o). \quad (10)$$

With only a minor loss of generality, we assume for this demonstration that $C_1^o = C_1^m = C_1$ and $C_2^o = C_2^m = C_2$, such that we may subtract (10) from (9) and arrive at a description of the difference between modeled and observed time rates of change of surface soil moisture:

$$\frac{\partial \theta_g^m}{\partial t} - \frac{\partial \theta_g^o}{\partial t} = \frac{C_1}{\rho_w d_1}(P_g^m - P_g^o) - \frac{C_1}{\rho_w d_1}(E_g^m - E_g^o) - \frac{C_2}{\tau}(\theta_g^m - \theta_g^o) + \frac{C_2}{\tau}(\theta_{\mathrm{geq}}^m - \theta_{\mathrm{geq}}^o). \quad (11)$$

This shows how the array of possible biases between modeled and actual (or observed) terms combine to yield a bias in the tendency of θ_g.

Because θ_{geq} is a function of θ_2 from (3), a bias between θ_2^o and θ_2^m will map directly into a bias between θ_{geq}^o and θ_{geq}^m, which will act, through the last term of (11), to create bias between the temporal derivatives of θ_g^o and θ_g^m. We assume, for this first demonstration, that $P_g^m \equiv P_g^o$ and $E_g^m \equiv E_g^o$, with the understanding that biases in surface soil moisture would also inject biases in bare soil evaporation, but that these biases will be minor in (11) relative to the direct influence of the moisture differences $(\theta_g^m - \theta_g^o)$ and $(\theta_{\mathrm{geq}}^m - \theta_{\mathrm{geq}}^o)$. With this assumption and the rearrangement of (11) we arrive at an estimate of the actual value of θ_{geq},

$$\theta_{\mathrm{geq}}^o = \theta_{\mathrm{geq}}^m - \frac{\tau}{C_2}\left(\frac{\partial \theta_g^m}{\partial t} - \frac{\partial \theta_g^o}{\partial t}\right) - (\theta_g^m - \theta_g^o). \quad (12)$$

This value of θ_{geq} is defined so as to provide a rate of water exchange across the bottom of the surface soil layer, such that the temporal tendency of the modeled θ_g matches the tendency of the observed value. In practice, we define a Δt_2 update interval (e.g., daily), and the finite difference expression of (12) provides the update value of θ_{geq} as

$$\theta_{\mathrm{geq}}^o(t_i) = \theta_{\mathrm{geq}}^m(t_i^-) - \frac{\tau}{C_2}\left(\frac{\theta_g^m(t_i^-) - \theta_g^m(t_{i-1}^+)}{\Delta t_2} - \frac{\theta_g^o(t_i) - \theta_g^o(t_{i-1})}{\Delta t_2}\right) - [\theta_g^m(t_i^-) - \theta_g^o(t_i)], \quad (13)$$

where the time is discretized as $t_i = t_{i-1} + \Delta t_2$, the superscript minus indicates the state variable value before the updating, and the superscript plus indicates the value after the updating at time t_i. In Figure 1 a schematic of this assimilation methodology is shown, with θ_g^m (solid line) being modified to match θ_g^o (dotted line) every Δt_2 and the different slopes owing to a bias in θ_{geq}. Noting that $\theta_g^m(t_i^+) \equiv \theta_g^o(t_i)$, (13) reduces to

$$\theta_{\mathrm{geq}}^o(t_i) = \theta_{\mathrm{geq}}^m(t_i^-) - [\theta_g^m(t_i^-) - \theta_g^o(t_i)]\left(\frac{\tau}{C_2 \Delta t_2} + 1\right). \quad (14)$$

Finally, from θ_{geq}^o and an inversion of (3) it is possible to estimate the corresponding root zone soil moisture value θ_2^o, and adjust periodically (e.g., each day) the simulated root zone soil moisture θ_2^m to match this value.

In summary, the proposed assimilation procedure is triggered by the availability of state variable observations at a time increment of Δt_2 and is executed through updating (1) the surface soil moisture θ_g^m to match the observation θ_g^o and (2) the root zone soil moisture θ_2^m using θ_2^o given by the dynamic retrieval of (14) and (3).

To limit the possible effect of measurement error (or noise) in θ_g^o inducing lasting shocks in the time series of θ_2^m, we limit the allowed percent change to θ_2^m at any single assimilation step to 10% of the modeled value of θ_2^m. Future work will deal more formally with measurement errors. We explore the performance of this assimilation protocol in the context of in situ field data collected at an experimental catchment in southern Ireland.

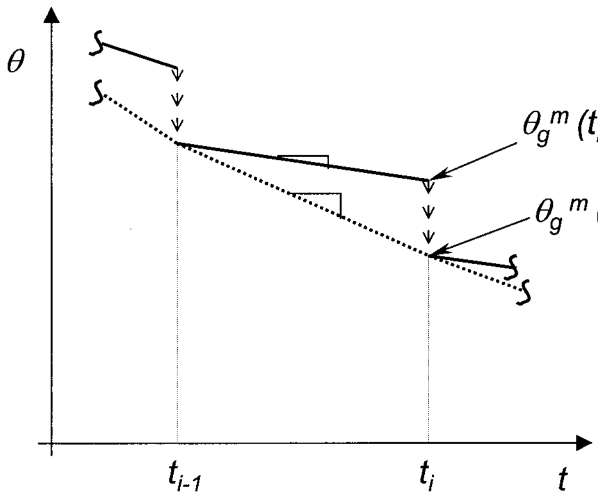

Figure 1. Schematic of the assimilation procedure. The modeled surface soil moisture θ_g^m is shown as a solid line, and the observed surface soil moisture θ_g^o is shown as a dotted line. The superscript minus indicates the modeled state before updating, and the superscript plus indicates the state after the updating.

3. Field Data

3.1. Experimental Site

The 15 Ha hillslope research field is at the headwater of the 98 km^2 Dripsey catchment 25 km northwest of the city of Cork, Ireland. The research field is an agricultural grassland at an elevation of 200 m above sea level (masl), with a gentle slope of 3% grade. The soil profile includes a top layer (5–10 cm thick) that is heavy in organic material (hummus) overlaying a sandy loam subsoil layer of 45 cm thickness. The grass heights vary through the year from 5 to 40 cm [*Albertson and Kiely*, 2001]. The local climate is temperate and humid, moderated by the warm influence of the Gulf Stream. Mean annual precipitation in the Cork region is ~1200 mm. The rainfall regime is characterized by long duration events of low intensity (typically less than ~3 mm h^{-1}) throughout the year. Less frequent, short-duration events of high intensity ($O(10^1)$ mm h^{-1}) occur mainly in summer.

3.2. Data Set

Hydrological and meteorological variables were measured continuously at this site for a 183 day period commencing early in 1998. Rainfall, air temperature, humidity, wind speed and direction, net radiation, soil heat flux, and soil temperature measurements were recorded on a 20 min averaging period. Soil moisture was monitored with time domain reflectometry (TDR) probes (Campbell CS615) installed horizontally at the depths of 2, 10, 20, 30, 40, 50, and 60 cm, with calibration based on intermittent gravimetric soil moisture measurements.

Table 1. Parameter Values Used in the SVAT Model for the Cork Experimental Site

Parameter	Description	Value	Source[a]
$K_{s,2}$	whole soil depth average value of the saturated hydraulic conductivity	10^{-7} m s^{-1}	cal.
$\theta_{s,2}$	whole soil depth average value of the saturated soil moisture content	0.50	obs.
$\lvert\psi_{s,2}\rvert$	whole soil depth average value of the air entry soil tension	0.30 m	R1982
b_2	whole soil depth average value of the slope of the retention curve in logarithmic space	4.90	C1978
$K_{s,g}$	surface layer value of the saturated hydraulic conductivity	2.4×10^{-5} m s^{-1}	obs.
$\theta_{s,g}$	surface layer value of the saturated soil moisture content	0.52	obs.
$\lvert\psi_{s,g}\rvert$	surface layer value of the air entry soil tension	0.36 m	R1982
b_g	surface layer value of the slope of the retention curve on logarithmic profile	5.39	C1978
θ_{wilt}	wilting point	0.13	D1977
θ_{fc}	field capacity	0.20	D1977
f_v	fraction of vegetation	1.00	A2001
$r_{s,\min}$	minimum stomatal resistance	150 s m^{-1}	A2001
LAI	leaf area index	2 m^2 m^{-2}	A2001
z_{om}	roughness length for momentum	0.03 m	A2001
z_{os}	roughness length for scalars	$z_{om}/7.4$ m	B1982
d_2	depth of root zone	0.40 m	obs.

[a]Sources are defined as follows: obs., approximate value from field observations; cal., value from model calibration; A2001, *Albertson and Kiely* [2001]; D1977, *Donahue et al.* [1977]; B1982, *Brutsaert* [1982]; R1982, *Rawls et al.* [1982]; C1978, *Clapp and Hornberger* [1978].

3.3. SVAT Parameters

The stratified soil profile is modeled [*Montaldo and Albertson*, 2001] using different soil parameters for each layer (Table 1). The saturated hydraulic conductivity of the surface layer was measured using a double-ring infiltrometer. The remaining soil parameter values were derived from literature data [*Clapp and Hornberger*, 1978; *Rawls et al.*, 1982] on the basis of measured soil texture for the profile. The root zone depth (d_2) was estimated at 0.4 m on the basis of visual inspection of soil cores, and d_1 was taken to be 10 cm. In Figure 2a the measured soil moisture data in the surface and root zone layers (with appropriate depth averaging across probes) are reported along with the rainfall time series. Figure 2b shows the comparison between observed and simulated soil moisture values using the model (no assimilation) with the parameters of Table 1. Using a $k_{s,2}$ of 10^{-7} m s^{-1} in the original (no assimilation) model provides the lowest RMSE for θ_2 over the entire data set (RMSE of 0.028), including reasonable performance during the dry excursions. Note that a fraction of the analysis that follows makes use of these "best estimate" parameters, while the remainder injects deliberate error into soil hydraulic properties. In all cases, explicit mention in made of the parameters being used.

The proposed assimilation scheme is tested both for the entire data set of 183 days and for four shorter periods of 30 days each, which were selected to explore the assimilation skill

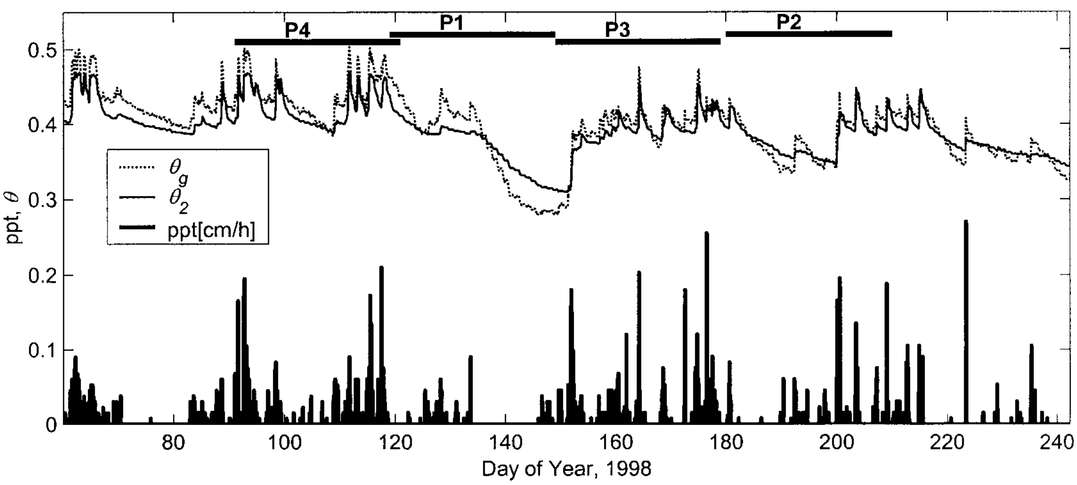

Figure 2a. Measured surface (θ_g) and root zone (θ_2) soil moisture and recorded rainfall time series from March 1, 1998. Four short 30 day periods that are the focus of certain analyses are marked (P1–P4) and defined in Table 2.

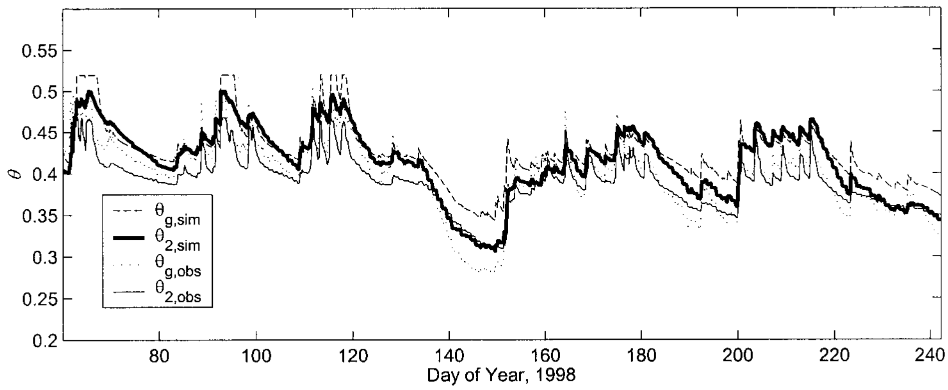

Figure 2b. Comparison of predicted and observed surface soil moisture ($\theta_{g,\text{sim}}$ and $\theta_{g,\text{obs}}$) and predicted and observed root zone soil moisture ($\theta_{2,\text{sim}}$ and $\theta_{2,\text{obs}}$) using model parameters from Table 1.

in distinctly different hydrometeorological conditions. The four short periods (P1, P2, P3, and P4) are described in Figure 2a and in Table 2.

4. Long-Term Assimilation Results

The availability of such a long data set (183 days) permits a broad test of the reliability of the proposed operational assimilation system. Taking the TDR measurements of θ in the top 10 cm as a proxy for the remote sensing observed surface soil moisture, the assimilation scheme consists of updating θ_g^m with θ_g^o and updating θ_2^m with the θ_2^o obtained from (12), subject to the operational adjustment limit described above to limit the shocks from possible measurement errors.

4.1. Evaluation Relative to the Hydrostatic Assumption

The presence of particularly wet hydrometeorological conditions (precipitation $\gg$ evaporative demand) during the observation period (Figure 2a) suggests that the hydrostatic hypothesis may be suitable to this data set for the retrieval of root zone soil moisture [e.g., *Jackson*, 1980]. The reliability of the hydrostatic hypothesis for the Cork data set is supported by Figure 3, where the measured root zone moisture content (points) and the hydrostatic estimates (line) are plotted against the measured surface moisture values. Note that the hydrostatic root zone values are lower than the corresponding surface layer values under dry conditions because of the vertical inhomogeneity of the soil hydraulic properties (taken into account in the hydrostatic calculations). From Figure 3 it is apparent that the hydrostatic assumption is reinforced by the measured data over a range of surface moisture values ($0.37 < \theta_g < 0.47$) that brackets a large fraction of the observational period (see Figure 2a). For the few short events with $\theta_g > 0.47$ the hydrostatic assumption overestimates θ_2, and for low θ_g values it underestimates θ_2. So, while there is good reason to expect the hydrostatic approach to work well under these conditions, there is also reason to believe that under significantly drier conditions than those encountered here, with logically large matric potential gradients in the vertical, the hydrostatic approach will fail.

A preliminary evaluation of the proposed assimilation protocol performance is performed by comparing its predictive skill to the simple retrieval based on the hydrostatic assumption. To avoid confusion between assimilation (or retrieval) performance and the general SVAT model performance, we employ here a "synthetic case" in which synthetic observations of surface soil moisture values (θ_g^o) are taken from the simulated values using the model with the best estimate parameters from Table 1. With this approach we can focus on the relative abilities of the assimilation approaches to compensate for misspecification of hydraulic properties (or initial conditions). Table 3 shows the RMSE in θ_2 simulations for three model approaches: no assimilation, assimilation of θ_g by hard updat-

Table 2. Hydrometeorological Characteristics of the Four 30 Day Periods

Period	Days	Precipitation, mm	Potential Evapotranspiration, mm
P1	119–149	25	71
P2	180–210	96	63
P3	149–179	139	60
P4	91–121	169	45

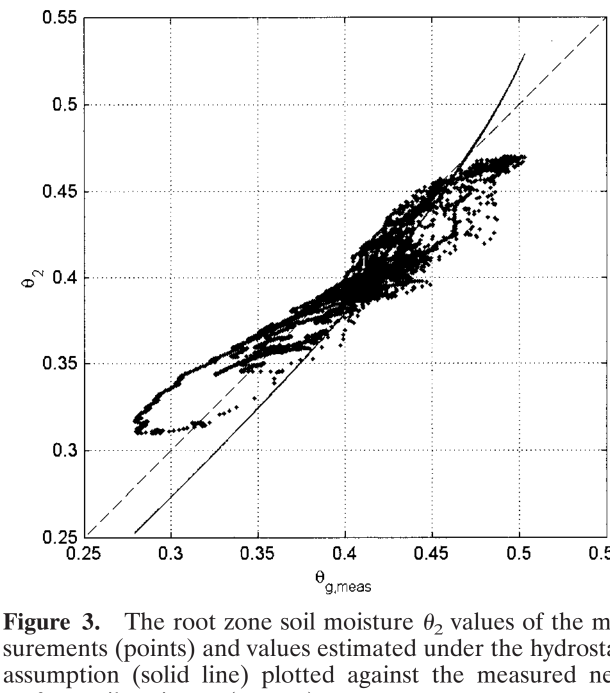

Figure 3. The root zone soil moisture θ_2 values of the measurements (points) and values estimated under the hydrostatic assumption (solid line) plotted against the measured near-surface soil moisture ($\theta_{g,\text{meas}}$).

Table 3. Comparison of the Model Results From the Original ISBA Model (Case 1), Assimilation of θ_g^o and θ_2^o Using the Proposed Approach Based on (12) (Case 2), and Assimilation of θ_g^o and θ_2^o Using the Hydrostatic Equilibrium Hypothesis (Case 3) (Using "Synthetic" Data)

$k_{s,2}$	Case	RMSE
10^{-7}	1	0.000
10^{-7}	2	0.002
10^{-7}	3	0.012
10^{-9}	1	0.082
10^{-9}	2	0.004
10^{-9}	3	0.013

ing and of θ_2 by the proposed approach using (14), and assimilation of θ_g by hard updating and of θ_2 by the hydrostatic assumption. In all three modeling formulations we used different soil parameters for the two layers. For the hydrostatic case this involved the extrapolation of a hydrostatic matric potential profile and local conversions to soil moisture based on the local soil properties of each layer. Of course, when the model parameters are kept the same as those used to generate the synthetic data, then the model (without assimilation) provides perfect agreement to the data (see Table 3). However, if we inject a two orders of magnitude error in $k_{s,2}$ (i.e., 10^{-9} m s^{-1}), then the no assimilation approach yields a considerable error (RMSE of 0.082). As also shown in Table 3, the hydrostatic assumption injects only a modest error (RMSE of 0.012) for the correct $k_{s,2}$ case, reinforcing the earlier statements that the vertical profile during this experiment is close to hydrostatic on average. However, for the biased $k_{s,2}$ case the proposed assimilation approach provides much greater accuracy than the hydrostatic case, suggesting that even under these wet conditions the proposed model is superior to the hydrostatic assimilation approach for long-term modeling in the presence of imprecise model parameters.

Motivation for data assimilation stems from a need to constrain model drift over long temporal integrations and the emerging availability of distributed observations of some model state variables. The aim is to improve model performance, especially when the model is a coarse representation of the underlying physics and is not directly calibrated. For this reason we progress to analyze the assimilation scheme's sensitivity to the soil properties, then we explore the influence of the soil moisture initial conditions, and finally, we explore the impact of assimilation frequency on predictive skill.

4.2. Sensitivity of the Assimilation Protocol to Errors in Specified Soil Hydraulic Properties

It is important that the approach be robust in the presence of uncertain parameters, as is typically the case for operational applications of distributed models over large regions. Two model approaches are compared using the field-observed soil moisture data: (1) no assimilation, and (2) assimilation of θ_g by hard updating and of θ_2 by the proposed approach using (14). Here we use the measured surface data for assimilation; the synthetic analysis was limited to section 4.1.

The models are employed first using the soil parameters of Table 1, which represent our best reasonable estimates, and then in additional cases using saturated hydraulic conductivity values for the deep soil, $k_{s,2}$, that vary over a wide range. The assimilation frequency is fixed at 1 day^{-1} for this soil properties analysis. The initial conditions of θ_g and θ_2 are set equal to the measured soil moisture values to isolate the effects of soil properties knowledge on data assimilation importance. Uncertainties in the initial conditions of the state variables are addressed later.

As an example of the temporal results from the two model formulations, the case with a low value of $k_{s,2}$ ($= 10^{-8}$ m s^{-1}) is shown in Figure 4. With this erroneously low $k_{s,2}$ value we note that the base model predicts moistures that are consistently wetter than the measurements, as the drainage is underestimated. The proposed dynamic assimilation approach provides marked improvement to the model performance. The comparison of the simulated and observed θ_2 values is reported through scatterplots in Figure 5. The average bias in the predictions (i.e., shift along vertical axis) is removed by the proposed approach, with an error in the slope resulting from the effect of the inexact soil parameters on the retrieval algorithms (e.g., through errors in C_2). The bulk of the data points are in the range where agreement is excellent, leading to the low RMSE of 0.034.

The results of the sensitivity analysis of the proposed implementation to misspecification of $k_{s,2}$ are summarized in Figure 6. Recall that our best estimate for conductivity is $k_{s,2} = 10^{-7}$ m s^{-1}. We vary the value of $k_{s,2}$ over five orders of magnitude in a series of model runs. As expected, the basic model (without assimilation) performance deteriorates significantly for even moderate errors in $k_{s,2}$. When the soil parameters and initial conditions are correctly specified, the assimilation offers no real improvement in model skill. However, the assimilation approach is much more robust than the original model with respect to misspecification of $k_{s,2}$, providing low values of RMSE ($<$0.04) for a wide range of values of $k_{s,2}$. Interestingly, the assimilation skill is more robust for large underestimation than for overestimation of $k_{s,2}$. This is because the dynamics of θ_2 resulting from drainage are fast for the high $k_{s,2}$ cases, resulting in large errors for the time periods between assimilation steps (i.e., within Δt_2). In summary, the assimilation improves performance over the base model for all but a narrow range of $k_{s,2}$ values around the correct value, suggesting that the assumption that modeled and real C_1 and C_2 are equivalent (leading up to (14)) is not too deleterious.

4.3. Sensitivity of the Assimilation Protocol to Errors in Soil Moisture Initial Conditions

A sensitivity analysis of the proposed assimilation approach to the soil moisture initial conditions is performed and reported in Figure 7. The assimilation performance is measured for soil moisture initial values equal to 30, 50, 75, and 100% of the initial observed values, using four values of $k_{s,2}$ (5×10^{-4}, 5×10^{-5}, 5×10^{-7}, and 5×10^{-9} m s^{-1}). The sensitivity analysis shows that the long-term model performance (with and without assimilation) is only slightly sensitive to initial conditions. This result is due to the combination of a long analysis period and plentiful precipitation. The frequent rain events tend to reset θ_2 to $\theta_{s,2}$, thus removing the memory of the inaccurate initial conditions. We explore this topic further in section 5 using short analysis periods representing different prevailing hydrometeorological conditions.

4.4. Sensitivity of the Assimilation Protocol to Assimilation Frequency

The sensitivity of model skill to the assimilation frequency is performed for the same series of $k_{s,2}$ values (5×10^{-4}, $5 \times$

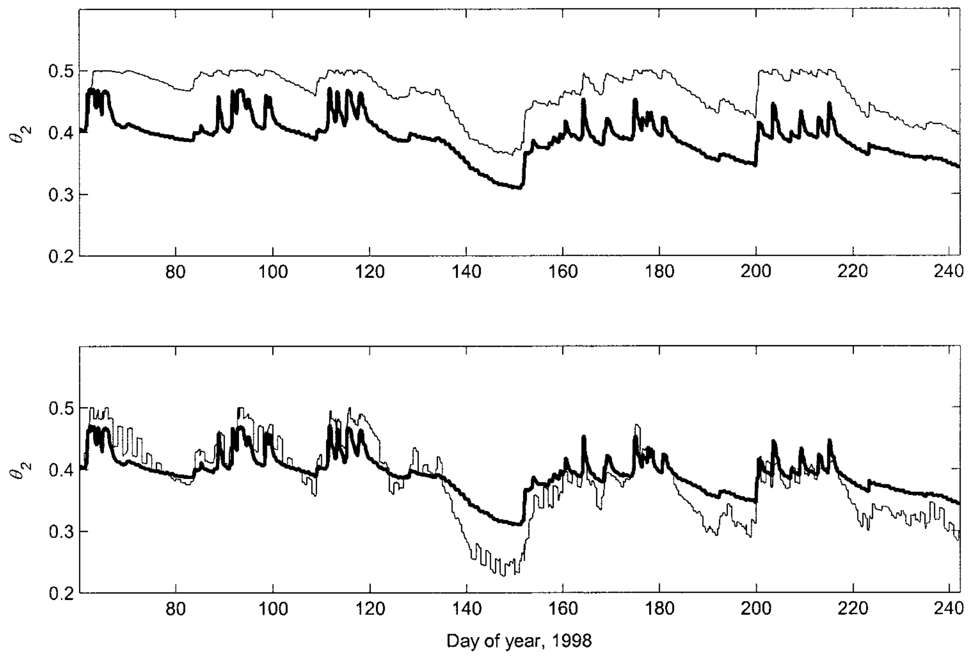

Figure 4. Soil moisture measurements and model predictions for two model approaches, using an intentionally low value of $k_{s,2}$ ($= 10^{-8}$ m s^{-1}). Observed root zone soil moisture θ_2 is marked with a thick line, and simulated θ_2 is marked with a thin line. The top panel is the base ISBA model case, and the bottom panel is the proposed assimilation approach. The assimilation approaches used reflect a daily update period.

10^{-5}, 5×10^{-7}, and 5×10^{-9} m s^{-1}). We explore update intervals of 3, 6, 12, 24, 72, and 120 hours in Figure 8. Sensitivity of the performance to assimilation frequency is noted for higher hydraulic conductivities, where the dynamics of soil water are active over short timescales, such that large errors can be developed between assimilation steps. The robustness of the model skill across a wide range of assimilation frequencies for an incorrect $k_{s,2}$ is encouraging, suggesting that infrequent model corrections are sustained by the internal model dynamics as needed for accurate predictions over long timescales.

5. Short-Period Assimilation Protocol Results

An analysis of the soil moisture assimilation system reliability is performed here for several shorter periods, each lasting 30 days. The periods (P1, P2, P3, and P4) represent a range of hydrometeorological conditions, going from a ratio of precipitation to potential evaporation (P/PET) of 0.35 for P1, with progressive increases to a ratio of 3.8 for P4. The characteristics of the periods are listed in Table 2 and referenced on Figure 2a. A daily assimilation interval and the value of 5×10^{-7} m s^{-1} for $k_{s,2}$ are used for this analysis. Here we perform a sensitivity analysis to inaccuracies in the specification of soil moisture initial conditions. Soil moisture initial conditions equal to 50, 75, and 100% of the observed values are specified for the model runs. Figure 9 shows the impacts of errors in initial conditions on the skill of the base model and the proposed assimilation approach for each period. As expected, the wet conditions of P4 render the simulation skill least sensitive to errors in the soil moisture initial conditions. Indeed, significant precipitation events, in particular at the start of the analysis period, erase the initial conditions such that the model (without assimilation) is able to simulate correctly the soil

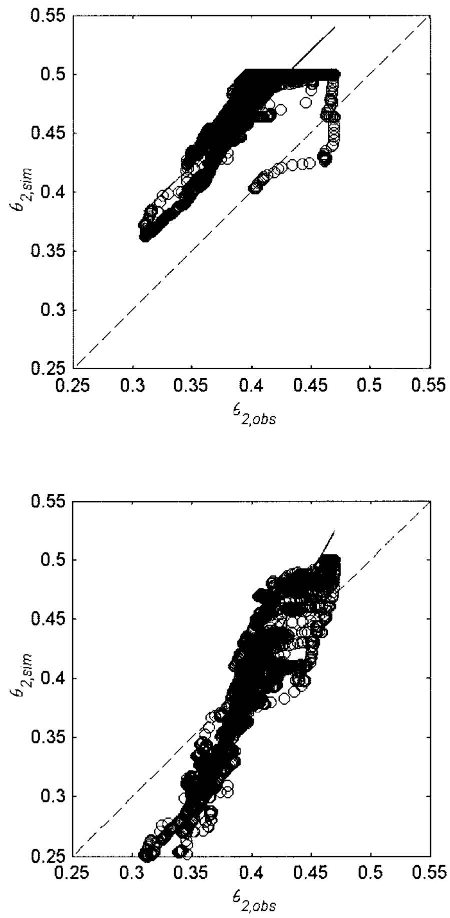

Figure 5. The root zone soil moisture results of Figure 4 as scatterplots in same order.

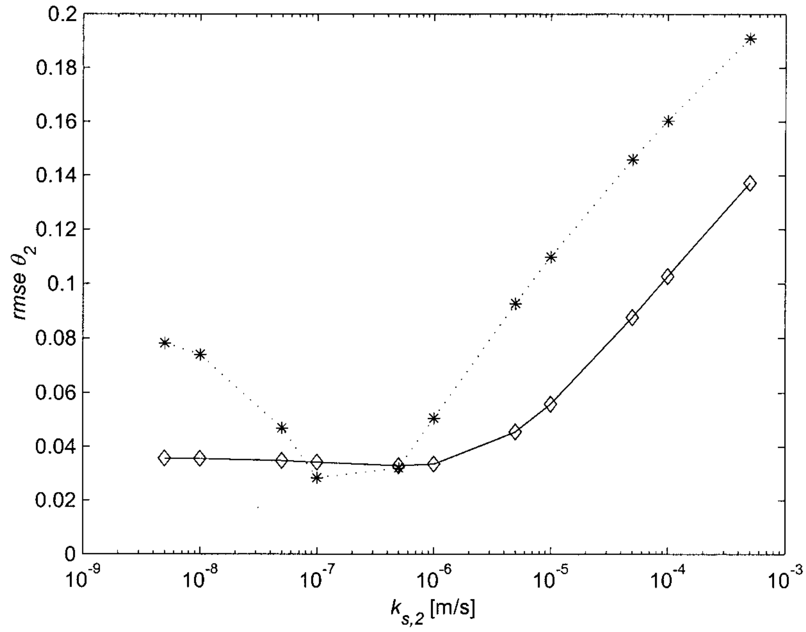

Figure 6. Root-mean-squared error (RMSE) of θ_2 model predictions plotted against assumed value of $k_{s,2}$ for the model runs. The lines reflect no assimilation (dotted line and asterisks) and assimilation of θ_g and θ_2 using the proposed approach based on (12) (solid line and diamonds).

moisture. For the drier periods the assimilation becomes more important in compensating for poor initial conditions.

The effects of general wetness or aridity on the model skill improvement from the assimilation protocol is measured by an assimilation efficiency, which we define as

$$\eta = \frac{\mathrm{RMSE}_o - \mathrm{RMSE}_a}{\mathrm{RMSE}_o}, \tag{15}$$

where RMSE_o is for the model without assimilation and RMSE_a is with the proposed assimilation approach. In Fig-

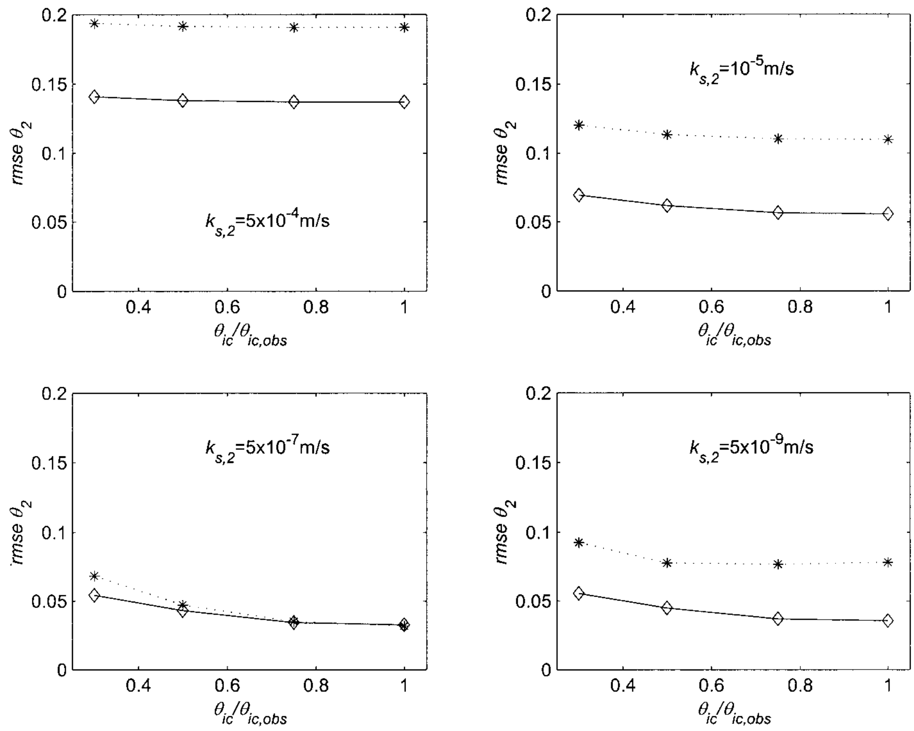

Figure 7. Sensitivity analysis of the root zone soil moisture assimilation to soil moisture initial conditions ($\theta_{2,ic}$) for several $k_{s,2}$ values. The no-assimilation model form is marked with a dotted line and asterisks, and the assimilation of θ_g and θ_2 using the proposed approach based on (12) is marked with a solid line and diamonds.

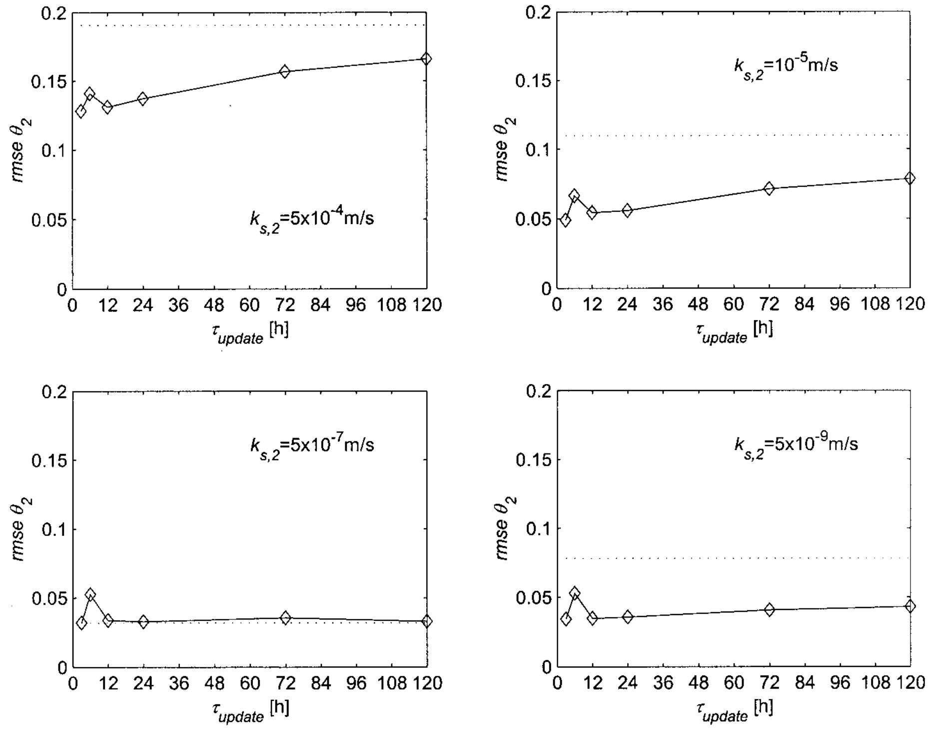

Figure 8. Sensitivity analysis to assimilation update intervals (τ_{update}) for several $k_{s,2}$ values. The no-assimilation model approach is marked by a dotted line, and the assimilation of θ_g and θ_2 using the proposed approach based on (12) is marked with a solid line and diamonds.

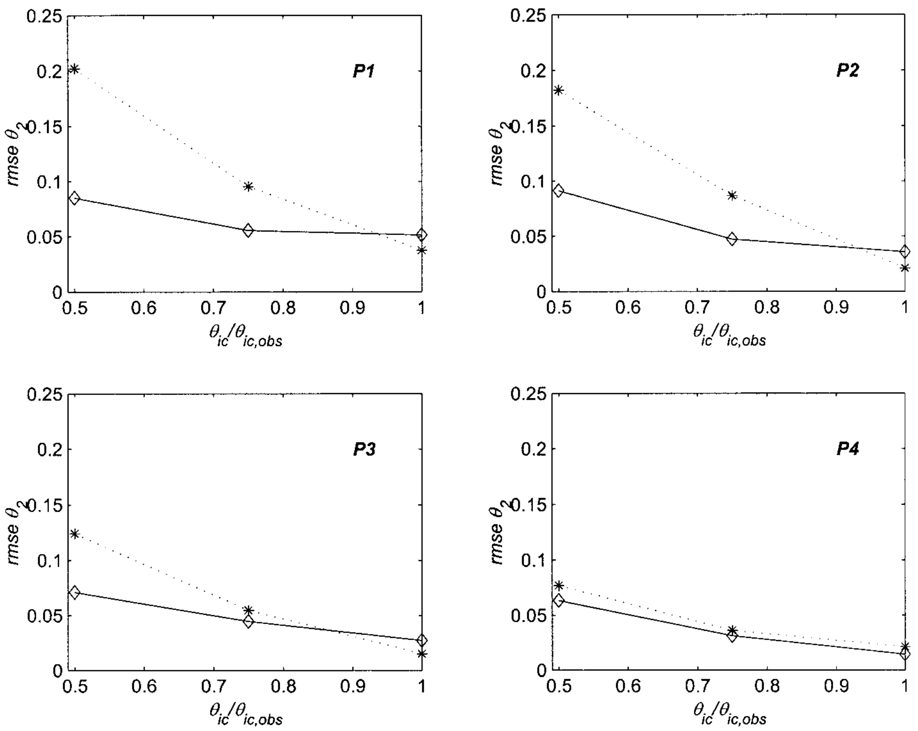

Figure 9. Comparison of the RMSE of the θ_2 models with and without assimilation versus the soil moisture initial condition ($\theta_{ic}/\theta_{ic,\text{obs}}$), using $k_{s,2}$ equal to 5×10^{-7} m s^{-1}, for the four periods (P1–P4) defined in Table 2. The no-assimilation model approach is marked by a dotted line and asterisks, and the assimilation of θ_g and θ_2 using the proposed approach based on (12) is marked with a solid line and diamonds.

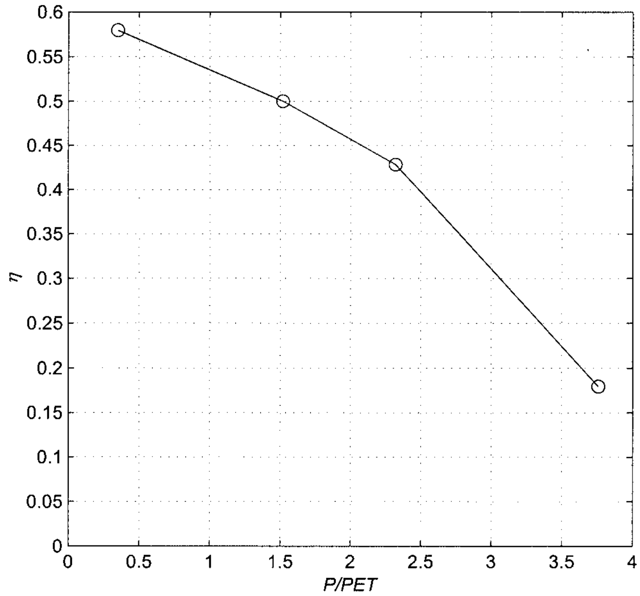

Figure 10. Efficiency η of the assimilation system versus the ratio between total precipitation and potential evapotranspiration (PET), P/PET, for the case with $k_{s,2}$ equal to 5×10^{-7} m s^{-1} and soil moisture initial conditions set to the 50% of the observed values.

ure 10, η is shown against the ratio between total precipitation and potential evapotranspiration (PET), P/PET, for each period for soil moisture initial conditions set to the 50% of the observed values. The η efficiency increases dramatically with decreasing P/PET.

6. Conclusions

The development of a basis for an operational assimilation protocol was described and tested. The results demonstrated that the approach is able to dynamically improve root zone soil moisture simulations based on the assimilation of near surface soil moisture observations, such as might be available from remote sensing platforms. The approach was motivated by the need to compensate for imperfections in model parameterization and specification of initial conditions.

We adopted the simple force-restore SVAT scheme for the operational assimilation system because it is parsimonious and reasonably accurate. The updating of only the surface soil moisture in these models has negligible value to the root soil moisture accuracy. Moreover, approaches based on a priori relationships between surface and root zone moisture contents are not expected to be robust over a wide range of hydrodynamic conditions, where the a priori relationships are violated in practice. For this reason, we presented an assimilation approach that is based on an analytical (and dynamical) relationship between surface and root zone soil moisture. The difference between observed and modeled time rates of change of surface soil moisture is analytically tied to a bias in the modeled moisture state of the lower root zone. The proposed approach is expected to perform well under arbitrary hydrometeorological conditions.

The availability of a long data series for the Cork experimental site permitted demonstration of the approach's effectiveness for both long periods (where initial states are not very important but model drift can be) and select short periods (where initial conditions can be important). An assessment of the impact of inexact soil hydraulic parameters on the model skill demonstrated that the proposed assimilation protocol maintains excellent soil moisture predictions over a three order of magnitude variability in the assumed hydraulic conductivity. The sensitivity analysis to the assimilation frequency highlighted that the procedure is significantly influenced by the updating period only under high hydraulic conductivity, such that the dynamics are fast enough to induce large errors in between assimilation steps.

Uncertainty in soil moisture initial conditions did not affect significantly the long-term soil moisture predictive skill for this wet experimental field. The importance of data assimilation to improving short-term (30 days) model skill was demonstrated to depend on hydrometeorological conditions. For periods with precipitation well in excess of evaporative demand the memory of initial soil moisture conditions is rapidly lost, whereas in drier conditions the model has more persistent memory and the assimilation has greater impact.

Future work is planned to cast the work presented here in a more formal assimilation context, where measurement and model errors will be treated simultaneously and optimally. The dynamical relationship between bias in time rate of change of surface moisture and bias in root zone status (14) is proposed to serve as the core of such an assimilation protocol.

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