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Towards soil property retrieval from space: Proof of concept using in situ observations

Ranmalee Bandara *, Jeffrey P. Walker, Christoph Rüdiger

Department of Civil Engineering, Monash University, Clayton 3800, Australia

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SUMMARY

Soil moisture is a key variable that controls the exchange of water and energy fluxes between the land surface and the atmosphere. However, the temporal evolution of soil moisture is neither easy to measure nor monitor at large scales because of its high spatial variability. This is mainly a result of the local variation in soil properties and vegetation cover. Thus, land surface models are normally used to predict the evolution of soil moisture and yet, despite their importance, these models are based on low-resolution soil property information or typical values. Therefore, the availability of more accurate and detailed soil parameter data than are currently available is vital, if regional or global soil moisture predictions are to be made with the accuracy required for environmental applications. The proposed solution is to estimate the soil hydraulic properties via model calibration to remotely sensed soil moisture observation, with in situ observations used as a proxy in this proof of concept study. Consequently, the feasibility is assessed, and the level of accuracy that can be expected determined, for soil hydraulic property estimation of duplex soil profiles in a semi-arid environment using near-surface soil moisture observations under naturally occurring conditions. The retrieved soil hydraulic parameters were then assessed by their reliability to predict the root zone soil moisture using the Joint UK Land Environment Simulator model. When using parameters that were retrieved using soil moisture observations, the root zone soil moisture was predicted to within an accuracy of 0.04 m^3/m^3, which is an improvement of $\sim$0.025 m^3/m^3 on predictions that used published values or pedo-transfer functions.

1. Introduction

The moisture content of soil is a key variable that controls the exchange of water and energy fluxes between the land surface and the atmosphere. This is because evaporation and transpiration are a function of the variability in soil moisture. Hence it plays a vital role in most environmental processes (Seneviratne et al., 2010), especially in the development of weather systems. Of the few important hydrological variables that can be directly observed, soil moisture has been declared as an Essential Climate Variable by the Global Climate Observing System (GCOS-107, 2006) and is therefore a reportable land surface parameter for contributing members. Because of the high spatial variability shown by soil moisture, monitoring very high resolution temporal changes globally, or even regionally, is not straightforward from both a logistical and an economic point of view. Both active and passive remote sensing methods are utilized in soil moisture monitoring, including the Advanced Microwave Scanning Radiometer-2 (AMSR2; C- and X-band) (Imaoka et al., 2010), Advanced Scatterometer (ASCAT; C-band) (Albergel et al., 2009) and Soil Moisture and Ocean Salinity (SMOS; L-band) (Kerr et al., 2010). However, current satellites are able to provide only the information for the top 1–5 cm, and consequently, there is still a great reliance on the soil moisture evolution predicted by land surface models (LSMs) to obtain soil moisture information for the top 1 m of soil, commonly referred to as the root zone.

LSMs are normally used to provide a boundary condition to weather and climate models, delivering the land surface feedbacks to the atmosphere. Hence, coupled land surface-atmosphere schemes must be able to predict the energy, water, and carbon exchanges, with explicit representation of vegetation and soil types. Yet, LSMs are often used uncoupled from atmospheric models and therefore require meteorological input data such as precipitation, temperature, radiation and so on, as well as parameters that represent the vegetation and soil of that area (Abramowitz et al., 2007). Soil hydraulic properties play a pivotal role as inputs to the LSM, regulating such things as infiltration and runoff. These parameters are normally derived from empirical equations that add value to basic information like field morphology, texture,

* Corresponding author. Tel.: +61 3990 54957 (O); fax: +61 3990 54944.
E-mail address: ranmalee11@gmail.com (R. Bandara).

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structure and pH, by translating them into estimates of other more difficult to measure soil properties, like the soil hydraulic properties. Yet, pedo-transfer functions cannot be extrapolated beyond the specific constraints, in terms of geomorphic region or soil type, under which it was developed (McBratney et al., 2002). Therefore, extrapolation over large areas yields crude estimates of soil hydraulic properties with large standard deviations (Vereecken et al., 1990; Vereecken et al., 1989), the accuracy of which deteriorates with the extent of the extrapolation, and thus adversely affects the accuracy of the model simulations. Thus, soil moisture estimates using LSMs typically suffer from physical parameterization, based on low-resolution and/or erroneous soil property information (Grayson et al., 2006). For example, De Lannoy and Reichle (2012) addressed the soil moisture biases of the GEOS-5 land data assimilation system by revising the global soil properties and soil hydraulic parameters that are used in the Catchment LSM through comparison against available in situ soil moisture measurements.

Remotely sensed soil moisture measurements can be used to address this soil hydraulic property estimation problem. However, most work to date has focused on utilizing synthetic simulations (Ines and Mohanty, 2008; Montzka et al., 2011), or observations on engineered soils (Burke et al., 1997a,b, 1998; Camillo et al., 1986; Ines and Mohanty, 2008; Santanello et al., 2007) (for a more detailed review of these studies refer to Bandara et al. (2013b)). Using a data assimilation approach, where model dynamics and remote sensing observations are merged, Qin et al. (2009) estimated both soil moisture and soil parameters simultaneously. They retrieved the soil texture and the soil porosity, concluding that the former contained large uncertainties when using different initial soil texture values, while the retrieval of soil porosity had relatively small uncertainties. Using an Ensemble Kalman Filter, Li and Ren (2011) explored the ability to calibrate the parameters of the van Genuchten–Mualem model through inverse modeling. They estimated three, four and five parameters and identified that the estimates of the two most important variables, saturated hydraulic conductivity and the shape parameter α, were improved. Moreover, they concluded that there were "many unsatisfactory estimates for the other three parameters". Pollacco and Mohanty (2011) showed that the high non-uniqueness of the inverted soil hydraulic parameters is due to their inter-correlation. Therefore, they proposed that a more accurate way of obtaining the saturated hydraulic conductivity and the air entry matric potential would be to scale them from point measurements. However, this was based on a numerical study for homogeneous soils, that this methodology would not be feasible for a large scale study under natural conditions.

Importantly, only a limited number of studies have focused on estimating soil hydraulic properties from soils under transient flow or naturally occurring boundary conditions. For example, the study by Dane and Hruska (1983) determined the hydraulic conductivity and soil water characteristic curves of soils undergoing drainage with the initial and boundary conditions known. Their methodology was initially tested for an engineered soil with known soil hydraulic characteristics, followed by a homogeneous clay loam soil. They concluded that the method should be applicable to heterogeneous soils, provided that both the boundary conditions and the water content profiles are well defined for each layer. However, this has not been tested, as prior knowledge of both the boundary conditions and the water content are rarely available in practice.

Using a measured time-series of soil water content at three different depths under natural boundary conditions, Ritter et al. (2003) estimated effective soil hydraulic properties utilizing the inverse parameter estimation method. Their study showed that when using laboratory determined soil hydraulic properties to simulate the water balance at field scale, inaccurate results were produced, and a 'trial and error' optimization did not yield objective results, leading to a poor fit of measured data. Consequently, they identified that efficient parameter estimation can be obtained only when an optimization algorithm is combined with the numerical model, demonstrating the feasibility of the inverse modeling approach to soil hydraulic property estimation of a soil column. Ritter et al. (2003) concluded that additional experimental data (drainage conditions, prior information of soil parameter data and so on) were needed to identify realistic parameters due to the ill-posed problem. An alternative approach, using a water injection experiment to derive effective soil parameters at field scale, has been tested by Ye et al. (2005) and Yeh et al. (2005). They applied spatial moments to 3-D snapshots of a moisture plume under impermanent flow conditions, to estimate the 3-D effective unsaturated hydraulic conductivity tensor. The effective hydraulic conductivities compared well with laboratory measured unsaturated hydraulic conductivity values. They concluded that the ratio of horizontal to vertical spreading of the plume, at varying moisture contents, confirmed the existing stochastic theories. Additionally, they also identified that the principal directions of the spatial moments varied as the moisture plume evolved through local heterogeneity, a feature that had hitherto not been recognized in the theories.

Despite these studies, all have focused on retrieving the soil hydraulic conductivity at saturation, and largely ignored the other soil hydraulic parameters. Consequently, the work presented in this paper focuses on retrieving all the important soil hydraulic parameters (Clapp and Hornberger exponent, hydraulic conductivity at saturation, soil matric suction at air entry, volumetric fraction of soil moisture at saturation, critical point, and wilting point), as shown in Table 1. In a former study (Bandara et al., 2013b), the authors developed a methodology for estimating the soil hydraulic properties of a heterogeneous soil column in a synthetic twin-experiment framework. According to this methodology, the soil hydraulic parameters were derived by calibrating an LSM to soil moisture observations, such as those which would be available from satellite observations. This study advances that work by applying the methodology to a field application with heterogeneous soil column under natural conditions. Given that this is a proof of concept study, it uses the more accurate and detailed in situ point measurements as opposed to satellite remotely sensed data. Satellite observed soil moisture observations were not used at this early stage due to their coarse resolution and the difficulty to validate results at those scales This study uses the Joint UK Land Environment Simulator (JULES) as the land surface model (Best et al., 2011; Clark and Harris, 2009; Clark et al., 2011), together with the Particle Swarm Optimization (PSO) method that is based on the complex collective behavior of individuals in decentralized, self-organizing systems, falling within the category of 'swarm intelligence' (Kennedy and Eberhart, 1995), and are discussed in detail under Section 3 of this paper.

2. Site and data description

The work presented in this paper focuses on three sites, Y2 (34.6548 S, 146.1103 E), Y5 (34.7284 S, 146.2932 E) and Y7 (34.8518 S, 146.1153 E). These sites are located near Yanco, New South Wales, Australia (as shown in Fig. 1), and form part of the OzNet soil moisture monitoring sites (Smith et al., 2012); http://www.oznet.org.au. The soil of the Yanco region is duplex, with horizon A being approximately 0.30 m deep. The dominant horizon A soil type at each location is loam, sandy loam and loam (Australian Bureau of Rural Science), respectively. The soil moisture has been measured continuously at depths of 0–0.05 m, 0–0.30 m, 0.30–0.60 m, 0.60–0.90 m (as shown in Fig. 2a) as the average over 30 min intervals using vertically installed Campbell Scientific

Table 1
Overview of the six soil hydraulic parameters and their physically feasible range, along with their respective notation, descriptive name, and unit where applicable.

Symbol	Parameter name and unit	Physically feasible range
b	Clapp and Hornberger exponent (–)	2–15
K_s	Hydraulic conductivity at saturation (mm/s)	0.0001–0.10
ψ_a	Soil matric suction at air entry (m)	−0.70 to −0.10
θ_s	Volumetric fraction of soil moisture at saturation (m^3/m^3)	0.10 – 0.60
θ_c	Volumetric fraction of soil moisture at critical point (for a soil suction of 3.364 m) (m^3/m^3)	0.10–0.50
θ_w	Volumetric fraction of soil moisture at wilting point (for a soil suction of 152.9 m) (m^3/m^3)	0.01–0.40

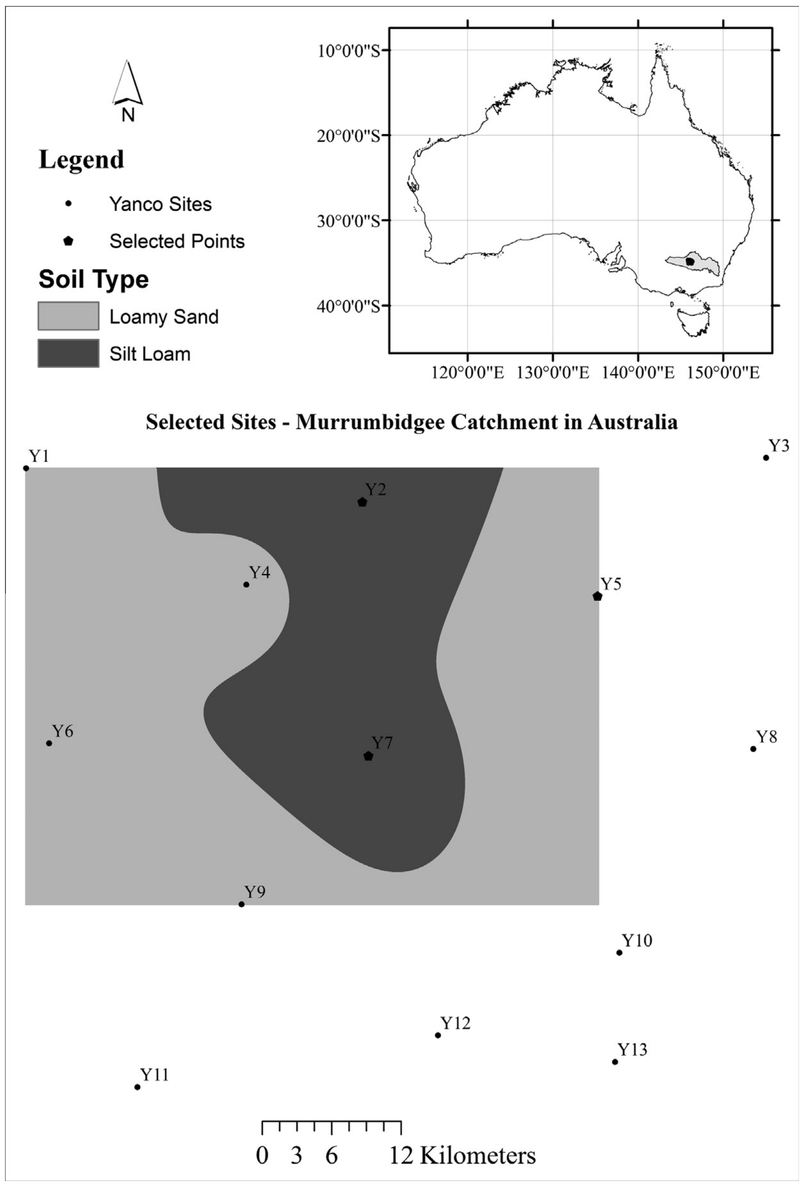

Fig. 1. Study site location together with the interpretation of the soil type based on the soil texture measurements made at the sites, Yanco area in the Murrumbidgee Catchment, Australia.

water content reflectometers and a Stevens Water surface soil moisture Hydraprobe, to provide integrated information along the profile, as described in Smith et al. (2012). The precipitation was measured by a tipping bucket rain gauge, with the cumulative rainfall recorded every 6 min (Smith et al., 2012).

This work focuses on the period between 2008 and 2010, as 2008 and 2009 were average years for the catchment (0.08–0.38 m^3/m^3 at the surface and 0.18–0.25 m^3/m^3 over the root zone) while 2010 was an exceedingly wet year (0.38 m^3/m^3 at the surface and 0.42 m^3/m^3 over the root zone). Hence, this time period covers the complete spectrum of dry to wet soil moisture conditions. The meteorological forcing data required by the JULES LSM (long and short wave radiation, wind speed, air temperature, humidity and pressure) were obtained from the automatic weather station located at the nearby Y3 (34.6208 S, 146.4239 E) station (Siriwardena et al., 2003), while precipitation and the specific soil and vegetation parameters were obtained from measurements at the focus site itself. To obtain initial conditions of soil moisture

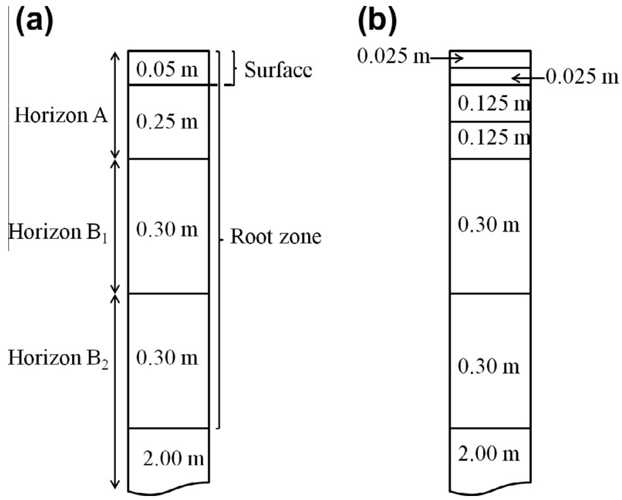

Fig. 2. The complete soil profile, as simulated by JULES. (a) The 3 horizons, A, B_1 and B_2, are shown with the surface and root zones as defined and (b) the thickness of each model layer.

and soil temperature corresponding to all seven model layers throughout the profile, model predictions commenced two years prior to the start of the focus period. The soil moisture of the pre-run was initialized at the point of saturation (0.55 m^3/m^3) for all layers, while soil temperature data were derived from in situ observations. The soil hydraulic parameters were obtained through four different sources; (i) experimental observations, (ii) published values (Rawls et al., 1982), (iii) calculated pedo-transfer function values from Cosby et al. (1984) using site specific particle size distribution data, and (iv) model calibration.

The experimental values were used for validation purposes, derived from a combination of field and laboratory measurements. The double-ring (twin-ring) infiltrometer method (Cook, 2002) was used for measuring the hydraulic conductivity at saturation (*Ks*) for the surface layer, while the well permeameter (McKenzie, 2002) was used to obtain the saturated hydraulic conductivity for the subsequent layers. A minimum number of two replicates of observations for each horizon were obtained at each site. The water level of the outer ring of the double-ring infiltrometer was kept constant while the change in water level of the inner ring was recorded every one minute. A similar procedure was followed when using the well permeameter, with measurements at 0.30 m, 0.90 m and 1.50 m depths. The equipment was dismantled when steady state flows were obtained. A minimum of three replicates of undisturbed soil core samples to a depth of 1.00 m were collected from all sites. These samples were then used in the laboratory to obtain the suction at air entry (ψ_a) using the filter paper method [ASTM D5298]. Accordingly, about ten samples were extracted from the core for each horizon using small metal rings. These were then subjected to different moisture conditions so as to acquire at least 8–10 data points along the soil water characteristic curve. The long term record of observed soil moisture was used to estimate the residual water content and the volumetric water content at saturation. The minimum and maximum observed values of the soil moisture over the period 2008–2011 were used as proxies for the volumetric water content at wilting point (θ_w) and at saturation (θ_s), respectively. These values are only used as a reference in discussing the results, in a manner similar to using the experimental soil hydraulic properties.

3. Modeling algorithms

This study uses JULES (Best et al., 2011; Clark and Harris, 2009; Clark et al., 2011) to simulate the time-series soil moisture profile corresponding to specified soil hydraulic parameters, with the particle swarm optimizer (Kennedy and Eberhart, 1995) used to 'retrieve' the best estimate of hydraulic parameters by matching predicted and observed soil moisture.

3.1. Land surface model (LSM)

JULES is a process based land surface model (LSM) that simulates the fluxes of carbon, water, energy and momentum between the land surface and the atmosphere, and is a derivative of the Met Office Surface Exchange Scheme (MOSES) (Cox et al., 1999). It can function either as a stand-alone model or coupled to a global circulation model. In a previous study, Bandara et al. (2011) assessed the performance of JULES and recommended it as a suitable model for this type of study.

The JULES LSM consists of four sub-models: soil, snow, vegetation and radiation (Best et al., 2011; Clark and Harris, 2009; Clark et al., 2011). Of these, the focus in this study is on the soil sub-model and the simulation of soil moisture. Herein, JULES is run with 7 soil layers of 0.025 m, 0.025 m, 0.125 m, 0.125 m, 0.30 m, 0.30 m, and 2.0 m thickness respectively (as shown in Fig. 2b), resulting in an overall soil depth of 2.9 m. Following extensive studies (which are not within the scope of the work presented in this paper), it was found that JULES was most stable with these layer thicknesses, and a timestep size not exceeding sixty minutes. When running JULES, it is necessary that the parameters and initial state values be correctly specified for each soil layer at the start of the simulation period. Consequently, initial state estimates were derived by setting all layer values to the point of saturation and undertaking a 2 year pre-run prior to the focus period (Bandara et al., 2013a – under review); the pre-run is repeated for each iteration of the model. Soil hydraulic parameters are governed by the Richards' equation and the van Genuchten (1980) constitutive relationships that are used in the calculation of soil moisture. Moreover, vegetation parameters are defined by a model tiling approach with up to nine surface types; broad leaf trees, needle leaf trees, C3 (temperate) grass, C4 (tropical) grass, shrubs, urban, inland water, bare soil and ice. Due to the prevailing surface conditions, the soil columns modeled in this study all have a single grass vegetation type.

The soil module of the JULES land surface model requires several parameters as inputs, and while it would be ideal to retrieve all of the soil parameters, it is not practical for several reasons. This is because some parameters play a more direct role in soil temperature simulation than on soil moisture, and the large number of parameters used by land surface models presents an equifinality issue. Moreover, the influence of some parameters on soil moisture simulation is comparatively higher than others. Hence, studies were conducted (Bandara et al., 2011; Bandara et al., 2013b) to identify the most sensitive parameters and to assess the capability of the LSM to retrieve such parameters. The soil hydraulic parameters retrieved in this paper include; (i) Clapp and Hornberger exponent, (ii) hydraulic conductivity at saturation, (iii) soil matric suction at air entry, (iv) volumetric fraction of soil moisture at saturation, (v) volumetric fraction of soil moisture at the critical point, defined as being equivalent to a soil suction of 3.364 m and, (vi) volumetric fraction of soil moisture at wilting point, defined as being equivalent to a soil suction of 152.9 m; see Table 1.

3.2. Particle Swarm Optimizer

The Particle Swarm Optimization (PSO) algorithm is based on the complex collective behavior of individuals in decentralized self-organizing systems, created through a population of individuals that interact both with each other and with the community. One benefit of using PSO is that it is easy to understand and to implement (Kennedy and Eberhart, 1995). However, the key feature of PSO is that it is less susceptible to getting trapped in a local minimum of the objective function since it is population-based, and thus has the capability to control the balance between the local and global search space (Engelbrecht, 2005b). This algorithm has been successfully utilized in a diverse range of applications, such as calibration of water and energy balance models (Scheerlinck et al., 2009), multi-machine power-system stabilizers (Abido, 2002), practical engineering designs (Hu et al., 2003), structural designs (Perez and Behdinan, 2007), and addressing generation planning problems (Kannan et al., 2004).

In the framework of PSO, particles are projected through a hyper-dimensional search space where changes to any selected particle's position are based on the social-psychological tendency of that individual to mimic the success of others (Engelbrecht, 2005b). Changes to the position of particles within the search space are therefore influenced by the experience and/or knowledge of its neighbor, in addition to its' own. The PSO algorithm comprises of three components; (i) the momentum, so that the velocity of the 'swarm' cannot change abruptly, (ii) the 'cognitive' or personal component (c_1), representing the particle's ability to learn from its own flying experience and fitness, and (iii) the 'social' component (c_2), representing the cooperation with other particles and thus learning from the flying experience of the group (Kennedy and Eberhart, 1995). One disadvantage of updating the velocity of the swarm is that it may become too high and cause particles to leave behind 'good' solutions, or too slow such that the search space is not explored adequately. Thus, to overcome this problem, Shi and Eberhart (1998) introduced an additional parameter, termed as the 'inertia weight' to control the velocity. The work presented in this paper uses the PSO code from Scheerlinck et al. (2009), with some slight modifications to facilitate parallelization.

The PSO algorithm uses four parameters: three inherent parameters and the population size defining the behavior of the swarm. Therefore, the first step of using the algorithm is to identify the 'best' parameters for driving the swarm. The size of the swarm was considered first, as larger swarms need a higher number of iterations to converge compared to smaller swarms, with very small swarms not yielding good solutions. Eberhart and Shi (2000) showed that a population size of 30 is adequate and this swarm size was adopted by Trelea (2003), Engelbrecht (2005b), Scheerlinck et al. (2009) and others. Hence, a swarm size of 30 particles was chosen for this study.

Shi and Eberhart (1998) identified that when w (the inertia weight) is less than 1, PSO is able to find the global minimum quite rapidly as it tends to act like a local search algorithm under this scenario, and targets an acceptable solution within the initial search space. However, when $w \geqslant 1$, the velocities of the swarm increase with time, the swarm diverges, and the particles fail to change direction towards regions with potential minima (Engelbrecht, 2005a). Additionally, Engelbrecht (2005a) states that $c_1 > c_2$ is more beneficial when applied to multimodal problems, as lower values of c_1 and c_2 yield smooth particle trajectories. Thus, the ranges that best fit the work presented in this paper were identified from existing literature, as discussed above, and the best combination of parameters for this problem was shown to be $w = 0.4$, $c_1 = 1.4$ and $c_2 = 1.3$ (Bandara et al., 2013b).

For this work, the root mean square error (RMSE) for the soil moisture prediction compared to observations has been utilized as the objective function of PSO. Additionally, parameters are restricted during the optimization process from moving beyond physically feasible values (as shown in Table 1). To further constrain the parameter from leaping to either end of the parameter space, a penalty was added to the RMSE, calculated between the true and simulated soil moisture. The imposed penalty was such that the parameter to be retrieved was given an initial approximate or best-guess value, and this value was allowed to vary three times the standard deviation of that parameter, thereby making the parameter space somewhat smaller and directing the optimization algorithm away from boundary values. The initial soil hydraulic parameters were based on the pedo-transfer function estimates using the soil texture information, with the standard deviations set according to the published values. However, PSO does not treat the initial values as a 'priori'; it is merely a value that contributes to the calculation of the objective function, the RMSE in this case.

4. Methodology

The objective of this study was to retrieve soil hydraulic parameters from soil moisture observations, and was approached in two steps. First, the soil hydraulic parameters for the complete soil profile were retrieved using both surface and root zone soil moisture observations, to provide a benchmark in the validation process. Second, only the surface moisture observations were used in retrieving the soil parameters for the complete soil profile. In both cases the retrieved parameters were validated against the experimentally observed parameter values. The predicted root zone soil moisture corresponding to observed, retrieved and published soil hydraulic parameters was also validated against the observed root zone soil moisture. For this proof of concept study, observational errors were not considered, and hence all field observations of soil moisture were assumed to be correct.

Though literature identifies the soils of Yanco as duplex, this study has allowed the soil profile to consist of three distinct horizons with potentially different soil properties; horizon A, horizon B_1 and horizon B_2 (as shown in Fig. 2a). This is because distinct differences in the particle size distribution were observed throughout the soil profile.

4.1. Benchmarking

Before assessing the proposed surface soil moisture calibration methodology for (i) retrieving the soil hydraulic parameters and (ii) more accurately predicting the root zone soil moisture, the capability of JULES to match the observed soil moisture measurements across the soil profile was tested. This not only shows shortcomings of JULES, but obtains a 'benchmark' for both retrieved hydraulic soil parameters and derived soil moisture predictions. Accordingly, PSO was used to retrieve soil parameters for the full profile, utilizing corresponding observed soil moisture data. In this setting, the simulated soil moisture is compared and soil parameters adjusted to best match the observed soil moisture for that particular soil layer, thus minimizing the objective function and yielding the 'best' values for each soil horizon.

The profile simulated by JULES has 7 layers of 0.025 m, 0.025 m, 0.125 m, 0.125 m, 0.300 m, 0.300 m and 2.000 m thickness, while field observations of soil moisture were for 4 layers of 0–0.05 m, 0–0.30 m, 0.30–0.60 m and 0.60–0.90 m depth from the soil surface. Consequently, weighted averages of the simulated soil moisture were used for comparison against the layer thicknesses of the field observations. The soil module of JULES utilizes eight parameters; Clapp and Hornberger exponent, volumetric fraction of soil moisture at saturation, critical point and wilting point, hydraulic conductivity at saturation, soil matric suction at air entry, dry heat capacity, and dry thermal conductivity. Results from the sensitivity study by Bandara et al. (2013b) show that of these eight parameters, the soil moisture simulations was mainly sensitive to six parameters only. Based on these findings, only the six soil parameters shown in Table 1 were estimated, as the soil moisture simulation was found to be most sensitive to changes in those parameters. It was also shown that the most suitable methodology for multi-parameter retrieval is a sequential approach, starting with the three most sensitive parameters (the volumetric fraction of soil moisture at critical point and at saturation, and the Clapp and Hornberger exponent) for all soil types, followed by the remaining three soil parameters. The main reason identified was that when the most sensitive parameters change, there is a significant change to the resulting soil moisture as opposed to changes in the less sensitive parameters. However, at least 3 cycles of sequential retrieval is completed to ensure that the best parameter combination is obtained.

4.2. Parameter retrieval with surface observations only

This study tests the hypothesis that root zone soil hydraulic parameters can be retrieved from surface soil moisture observations alone. A flow chart of the methodology is presented in Fig. 3. The surface soil moisture simulated by JULES was compared with that observed using in situ sensors, and the six soil hydraulic parameters listed in Table 1 retrieved for the complete soil profile using PSO, such that the objective function between the simulated and observed time-series was a minimum. The retrieved parameters were then compared with experimental observations, and the predicted root zone soil moisture compared with the observed root zone soil moisture. The initial LSM states were again obtained through a 2-year pre-run initialized at the point of saturation for each iteration. The objective function of PSO compares the simulated surface soil moisture from JULES with the corresponding soil moisture observations, and converging on the soil hydraulic parameters that minimize the RMSE between the two time-series. Given that the thickness of the observed surface layer is 0.05 m, the weighted average of the first two model layers in the simulation has been used.

The corresponding RMSE between the observed and simulated soil moisture, using the retrieved parameters, was calculated along with the Nash–Sutcliffe model efficiency coefficient (Nash and Sutcliffe, 1970). The Nash–Sutcliffe coefficient E can range from $-\infty$ to 1, with a perfect match between the modeled simulation and observation resulting in a value of $E = 1$. When $E = 0$, the model predications are no more accurate than simply using the mean of the observed data, whilst values of $E < 0$ can be interpreted as the observed mean being a better predictor than the model.

5. Results

The ability of JULES to match the observed soil moisture when using the entire profile of soil moisture observations as a constraint

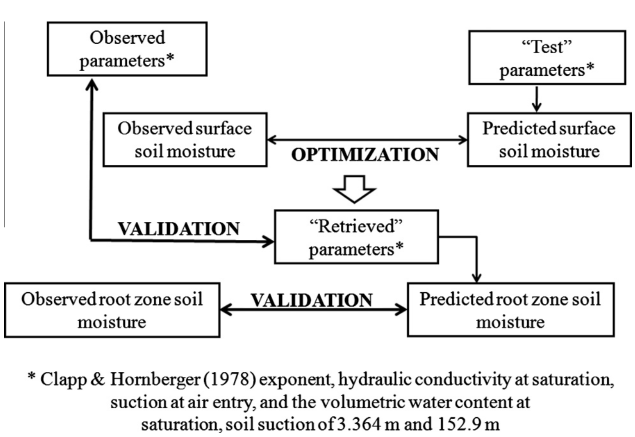

Fig. 3. Schematic of the parameter retrieval process using surface soil moisture observations.

was first determined. This provided the benchmark for subsequent retrievals when only surface soil moisture observations were used. Tables 2 and 3 provide a comparison of the published, retrieved and experimentally determined soil hydraulic parameters for sites Y2 and Y5 respectively. Of the three sites used in this study, results from only these two sites are presented, as both Y2 and Y7 provided similar results and had similar soil properties.

5.1. Benchmarking

When compared with experimentally observed soil parameters (Table 2), all retrieved benchmarking soil hydraulic parameters for Y2 were higher than the observed value, with the exception being the horizon A volumetric water content at saturation and critical point. The RMSE between the observed and predicted soil moisture (Table 4) was 0.049 m^3/m^3 and 0.014 m^3/m^3 for the surface and root zone when observed soil hydraulic parameters were used. These values were reduced to 0.038 m^3/m^3 and 0.020 m^3/m^3 when the retrieved soil hydraulic parameters were used. Thus the RMSE for the surface decreased by 0.011 m^3/m^3 while the root zone increased by 0.006 m^3/m^3 when optimized soil parameters were used to predict the soil moisture, as opposed to the experimentally observed soil parameters. The Nash–Sutcliffe efficiency for the surface was 0.684 when optimized soil hydraulic parameters were used, compared to 0.521 when observed soil hydraulic parameters were used. For the root zone, these values were 0.242 and −0.004 respectively. These values suggest that when experimentally observed soil hydraulic parameters were used, they provided a marginally more accurate root zone soil moisture prediction as compared to the optimized parameters. In either case the LSM provides little skill as compared to the mean value alone, suggesting that the model physics are in need of further improvement. This is highlighted further in Fig. 4, showing that JULES was unable to successfully capture the wet period towards the middle of 2009. At the same time, it should also be noted that the root zone soil moisture showed very little variation from the mean value. The soil moisture prediction with the observed soil parameters better captured the dynamics of the root zone, whereas the prediction with optimized parameters was unable to dry down as much as the field soil moisture. This resulted in the observed soil parameters better capturing the dry end but showing limitations in capturing the wet up. The scatter plots corresponding to the time series of soil moisture are depicted on the right-hand side of Fig. 4. It was seen that the soil moisture prediction using the optimized soil parameters was mostly wetter than the observed soil moisture, while the soil moisture prediction from the observed soil parameters underpredicted the observed soil moisture. Since the root zone was less dynamic, a concentration of points was observed at approximately 0.2 m^3/m^3, while the rest of the points were distributed horizontally. This horizontal distribution of points when the optimized soil parameters were used in the predictions was mostly due to the discrepancies in soil moisture for the first half of 2008 and 2009. When observed soil parameters were used in the soil moisture prediction, the discrepancies were spread throughout the year 2009, resulting in a flat distribution of points.

Similar to Y2, it is seen from Table 3 that the optimized parameters for Y5 were higher than those observed experimentally, with the exception being the volumetric soil moisture content at saturation and wilting point for horizons B_1 and B_2. The RMSE of the predictions using observed soil hydraulic parameters matched the observed surface soil moisture to within 0.033 m^3/m^3, while the optimization yielded a comparable accuracy of 0.035 m^3/m^3. However, the prediction with the optimized soil hydraulic parameters out-performed that with the observed soil hydraulic parameters for the root zone by a margin of 0.033 m^3/m^3. Similar results to Y2 were obtained for E, with the exception that a much

Table 2
Soil hydraulic parameters for horizon A (HA), horizon B_1 (HB_1) and horizon B_2 (HB_2) from; (i) experimental observation, (ii) Rawls et al., (iii) Cosby et al., (iv) Benchmarking optimization using surface and root zone soil moisture, and (v) optimized for the profile using surface soil moisture only. Site Y2.

Parameter	Observed		Rawls et al. parameters		Cosby et al. parameters		Optimized – benchmark			Optimized – surface only		
	HA	HB_1/HB_2	HA	HB_1/HB_2	HA	HB_1/HB_2	HA	HB_1	HB_2	HA	HB_1	HB_2
b	4.780	4.780	5.300	5.300	5.680	7.680	7.711	5.098	2.486	5.036	6.023	6.743
K_s	0.0017	0.0017	0.0072	0.0072	0.0040	0.0024	0.0029	0.0089	0.0040	0.0055	0.0054	0.0054
ψ_a	0.100	0.100	0.786	0.786	0.300	0.387	0.315	0.500	0.499	0.301	0.375	0.384
θ_s	0.410	0.400	0.485	0.485	0.446	0.458	0.395	0.437	0.390	0.421	0.350	0.443
θ_c	0.370	0.233	0.369	0.369	0.291	0.346	0.348	0.347	0.270	0.350	0.349	0.171
θ_w	0.050	0.180	0.179	0.179	0.149	0.210	0.240	0.237	0.145	0.095	0.186	0.170

Table 3
Soil hydraulic parameters for horizon A (HA), horizon B_1 (HB_1) and horizon B_2 (HB_2) from; (i) experimental observation, (ii) Rawls et al., (iii) Cosby et al., (iv) benchmarking optimization using surface and root zone soil moisture, and (v) optimized for the profile using surface soil moisture only. Site Y5.

Parameter	Observed		Rawls et al. parameters		Cosby et al. parameters		Optimized – benchmark			Optimized – surface only		
	HA	HB_1/HB_2	HA	HB_1/HB_2	HA	HB_1/HB_2	HA	HB_1	HB_2	HA	HB_1	HB_2
b	5.730	4.740	4.900	5.390	4.740	6.890	4.146	8.999	7.063	5.040	6.770	6.782
K_s	0.0018	0.00002	0.0725	0.0070	0.0104	0.0040	0.0043	0.0020	0.0069	0.0076	0.0061	0.0074
ψ_a	0.100	0.100	0.095	0.200	0.109	0.235	0.117	0.171	0.210	0.109	0.109	0.236
θ_s	0.400	0.420	0.435	0.451	0.406	0.438	0.413	0.450	0.450	0.450	0.351	0.430
θ_c	0.300	0.350	0.210	0.267	0.197	0.298	0.339	0.340	0.113	0.260	0.280	0.348
θ_w	0.010	0.180	0.096	0.132	0.088	0.171	0.187	0.149	0.108	0.095	0.172	0.186

Table 4
The root mean square error (RMSE) and Nash–Sutcliffe correlation coefficient (E), calculated between the observed and predicted surface and root zone soil using the observed, profile (benchmark) optimized, surface optimized, Cosby et al. and Rawls et al. soil parameters.

	Y2				Y5			
	RMSE (m^3/m^3)		E		RMSE (m^3/m^3)		E	
	Surface	Root zone	Surface	Root zone	Surface	Root zone	Surface	Root zone
Observed parameters	0.049	0.014	0.521	0.033	0.242	0.054	0.797	−1.184
Optimized parameters (benchmark)	0.038	0.020	0.684	−0.004	0.035	0.021	0.776	0.482
Optimized parameters (surface only)	0.037	0.027	0.645	−1.514	0.036	0.042	0.763	−0.398
Cosby et al. soil parameters	0.053	0.037	0.524	−3.935	0.035	0.044	0.751	−0.476
Rawls et al. soil parameters	0.038	0.044	0.688	−5.447	0.036	0.071	0.732	−2.153

larger value was obtained for the root zone in this instance, indicating that JULES was better able to capture the root zone dynamics of the sandy loam soil at this site as compared to the loam soil at Y2. However, Fig. 5 shows that JULES still struggled to capture the dynamics towards the end of 2010, despite being a close approximation for the remainder of the time sequence. Unlike in Y2 (Fig. 4), it was observed that the soil moisture predictions from both the observed and optimized soil parameters were quite similar, as shown from the scatter plot for the surface of Y5. As in the previous site, a flat distribution of points for the root zone was observed, mainly due to the large discrepancy between the observed and the predicted soil moisture.

Fig. 6 shows a comparison of the observed soil moisture for both the surface and root zone, against predictions using soil hydraulic parameters from (i) the most commonly used published values (Rawls et al., 1982), (ii) calculated values using the pedo-transfer functions of Cosby et al. (1984), (iii) optimized benchmarking values, and (iv) experimentally observed values. Fig. 6(a) corresponds to the soil moisture prediction curves using the parameter combinations shown in Table 2, while Fig. 6(b) is for the values in Table 3. From Fig. 6, it is observed that the predictions using the experimental and optimized soil hydraulic parameters best captured the moisture dynamics of the surface and root zone for both sites, when compared to parameters derived from either the published or pedo-transfer functions. From Table 4, it is observed that the highest RMSE for the root zone, 0.044 m^3/m^3 and 0.071 m^3/m^3 for Y2 and Y5 respectively, has been obtained for the soil moisture predictions using the Rawls et al. (1982) soil parameters. For the surface soil of Y2, the soil moisture predictions from Cosby et al. (1984) had the highest RMSE of 0.053 m^3/m^3. For both sites, under all four scenarios (except with the observed parameters for Y2 and the optimized parameters for Benchmarking of Y5), the root zone shows high negative values for E, thereby indicating that the root zone soil moisture predictions are worse than the observed mean values. The only time that the simulations using parameters from Rawls et al. (1982) and Cosby et al. (1984) showed a better match with observed soil moisture is for site Y2 during the wet period in 2009.

5.2. Parameter retrieval

This section addresses the main objective of this study, testing the feasibility of retrieving soil hydraulic parameters of a duplex soil column using soil moisture observations only. When compared with the experimentally observed and benchmark soil hydraulic parameters, it is observed that the optimized soil hydraulic parameters always lie between the two, sometimes closer to one or the other. For example, the surface suction at air entry and volumetric water content at the critical point for Y2 are close to the benchmarked values, while the same parameters at Y5 showed a closer match with the experimentally observed soil hydraulic parameters. As expected, Table 4 shows that the smallest RMSE for the surface soil moisture prediction at Y2 was obtained when optimized with the near-surface soil moisture alone, while the RMSE for the

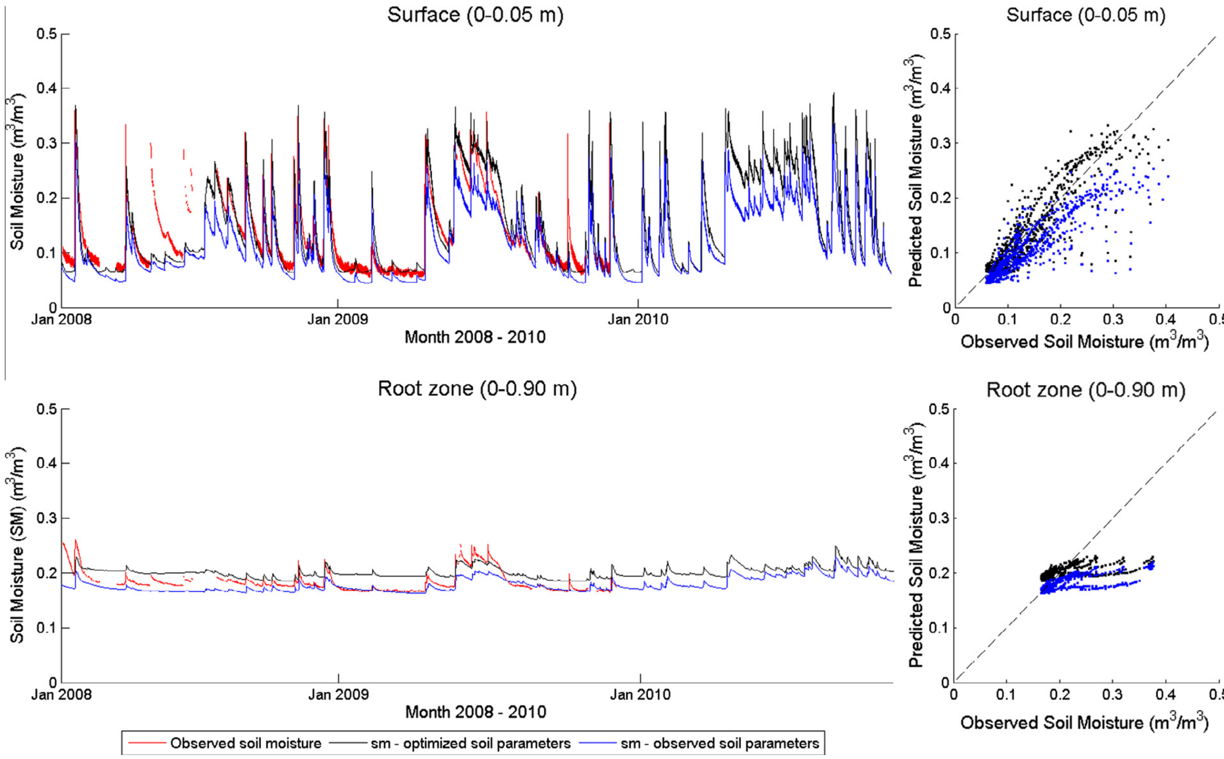

Fig. 4. Observed and predicted soil moisture for Site Y2 (silt loam soil) using (i) optimized and (ii) experimentally observed soil hydraulic parameters. Retrieved soil hydraulic parameters are from using both surface and root zone soil moisture observations to provide a benchmarking scenario. The corresponding scatter plots for the surface and root zone are shown on the left of the time series.

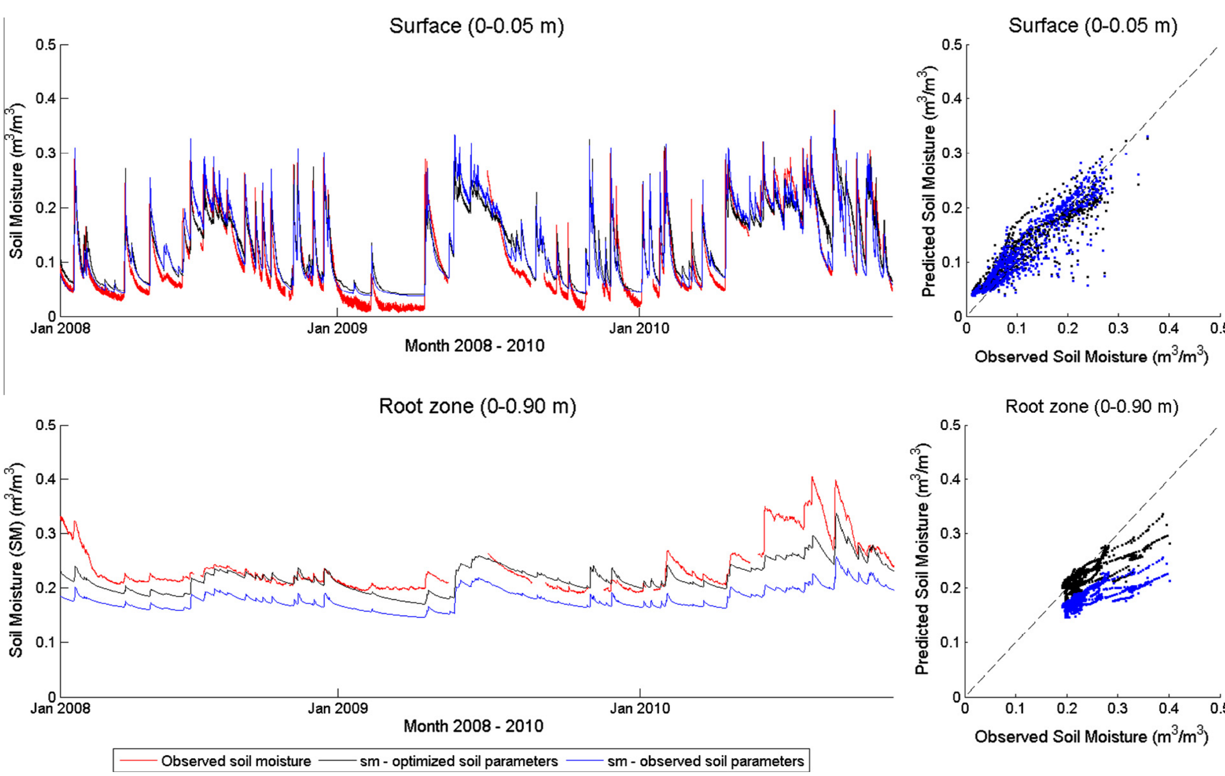

Fig. 5. Observed and predicted soil moisture for Site Y5 (loamy sand soil) using (i) optimized and (ii) experimentally observed soil hydraulic parameters. Retrieved soil hydraulic parameters are from using both surface and root zone soil moisture observations to provide a benchmarking scenario. The corresponding scatter plots for the surface and root zone are shown on the left of the time series.

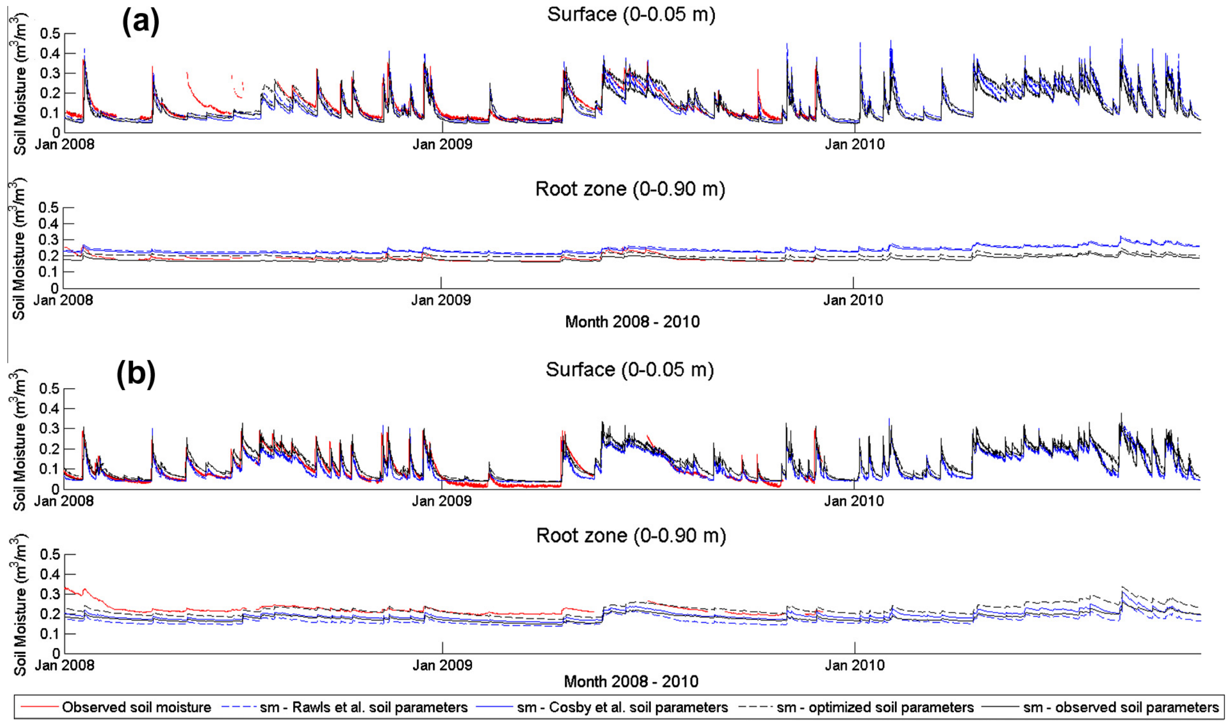

Fig. 6. Observed and predicted soil moisture for (a) Site Y2 and (b) Site Y5 using (i) Rawls et al., (ii) Cosby et al., (iii) optimized (Benchmark) and (iv) experimentally observed soil hydraulic parameters.

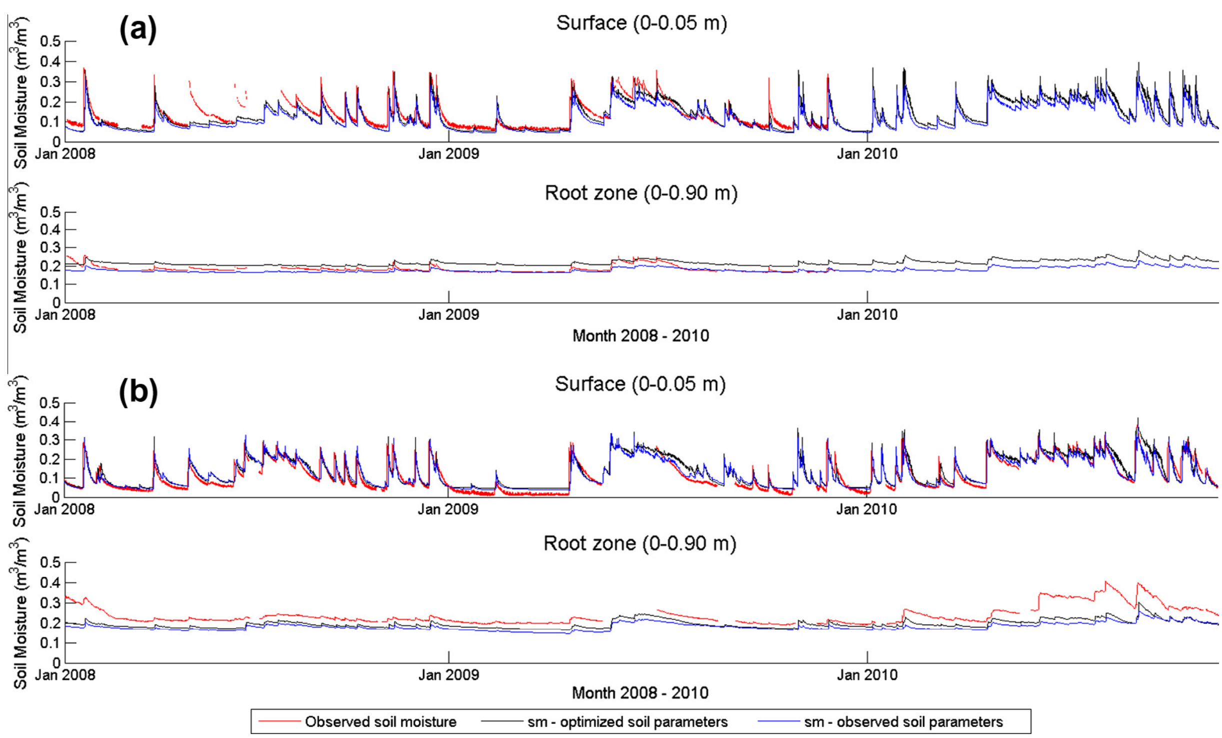

Fig. 7. Observed and predicted soil moisture for (a) Site Y2 and (b) Site Y5 from (i) experimentally observed and (ii) optimized soil hydraulic parameters, using surface soil moisture observations alone.

root zone soil moisture was much larger when compared to all the other retrieval scenarios. The root zone RMSE is twice as that when predictions are made using observed parameters and therefore, E is -1.514, indicating that the observed mean is a better predictor than the model. For site Y5, the root zone soil moisture predictions corresponding to the observed and optimized parameters using surface only observations did not yield positive values for E (only the benchmarking scenario had a positive E). Of the two, the surface only retrieval worked best with an RMSE of 0.042 m^3/m^3 and $E = -0.398$, as opposed to 0.054 m^3/m^3 and -1.184. However,

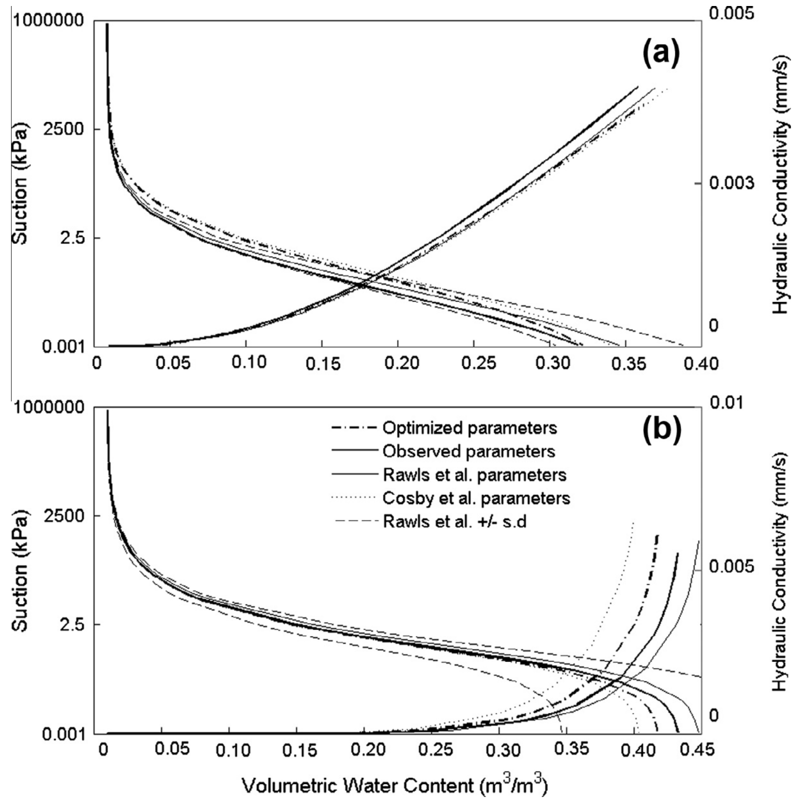

Fig. 8. The suction and hydraulic conductivity for (a) Site Y2 and (b) Site Y5, plotted against the volumetric water content of the soil.

the RMSE for the root zone between the observed soil moisture and prediction using surface moisture only retrieved parameters was twice that obtained through benchmarking.

It can be seen from Fig. 7(a) that the predicted soil moisture using observed soil parameters is most able to capture the dynamics of the root zone of Y2. Fig. 7(b), corresponding to Y5, shows that neither predictions are able to match the root zone soil moisture dynamics. From the same table, it is observed that the root zone RMSE corresponding to Cosby et al. (1984) and Rawls et al. (1982) for Y2 (0.037 m^3/m^3 and 0.044 m^3/m^3) are significantly larger than the RMSE obtained when only surface observations are utilized to retrieve soil parameters for the complete soil profile (0.027 m^3/m^3). Site Y5 performs in a similar manner. The E corresponding to the root zone when using either Cosby et al. (1984) or Rawls et al. (1982) is a large negative number when compared with either experimental or optimized parameters in the soil moisture prediction (e.g. −3.935 and −5.447 as opposed to 0.242 and −0.004/−1.154 for Y2). Therefore, when optimized parameters from the surface-only retrieval were used, the soil moisture RMSEs for the surface and root zone were almost equivalent to the 'best' results, which were obtained from benchmarking. This degradation is almost zero for the surface (0.001 m^3/m^3), less than 0.02 m^3/m^3 for the root zone, and a significant improvement over using pedo-transfer functions (approximately 0.02 m^3/m^3 for both the surface and root zone) or published values (approximately 0.03 m^3/m^3 for the root zone). It is also observed that the soil moisture predictions from optimized parameters using surface-only observations performed no worse than if experimental values were used. This is in vivid contrast to using either pedo-transfer functions or published values, which resulted in degraded model performances.

Fig. 8 shows the soil water characteristic curves (SWCC) obtained through the laboratory experiments together with the hydraulic conductivity curves. These are compared with those derived from the parameter combinations shown in Tables 2 and 3, for site Y2 and Y5 respectively. While all curves are within the standard deviation of the parameters given in Clapp and Hornberger (1978), the SWCC for the optimized parameters corresponding to Y2 sits closer to the SWCC of Cosby et al. (1984) parameters than to the observations. However, curves of the optimized parameters match closely with curves corresponding to the observed parameters for Y5. It is also observed that the published values and pedo-transfer functions encompass the optimized and observed parameters, illustrating the large amount of uncertainty in using these approaches.

6. Discussion and conclusions

This study showed that the JULES LSM was able to predict the soil moisture evolution to within 0.04 m^3/m^3 of observed surface and root zone soil moisture, providing the soil hydraulic properties were experimentally observed or calibrated using the soil moisture distribution across the profile. Any errors in observed soil moisture and/or precipitation observations were neglected, with the error assumed to be solely from the model predictive capability (i.e. its underlying physics). However, it was observed that model predictions were not able to perfectly match the field observed soil moisture, even using experimentally observed or calibrated (using the entire soil moisture profile) soil hydraulic parameters, and that the Nash Sutcliffe coefficient was typically low for the root zone soil moisture prediction, indicating a deficiency in the model physics that needs further investigation.

When using the surface soil moisture observations alone to retrieve the soil hydraulic parameters, the RMSE of surface soil moisture prediction was equivalent to that for the benchmarking case, which used the entire soil profile as a constraint, while the predicted root zone soil moisture was not as good as that of the benchmark. It was also observed that the optimized soil hydraulic parameters using near-surface soil moisture alone out-performed the soil moisture predictions (by approximately 0.02 m^3/m^3 for the surface and 0.03 m^3/m^3 for the root zone) using the published values of Rawls et al. (1982) and pedo-transfer functions of Cosby et al. (1984). It is therefore concluded that the use of soil moisture observations to retrieve soil hydraulic parameters for a duplex soil column should lead to an improvement on prediction skill when compared to the current approach of using published values. Thus, this method should be explored for large scale applications using soil moisture observations from satellite.

In this proof of concept study using in situ observed data, it has been assumed that the data are perfect at the point location. This was because the focus of the paper was to show the feasibility to retrieve meaningful parameters for the complete soil profile of a heterogeneous column of soil, using only the near-surface soil moisture observations. Satellite observed soil moisture observations were not used at this early stage due to its coarse resolution and difficulty to validate. In this study, many parameters corresponding to other model modules have been fixed, with only six parameters being retrieved. Hence, some of the discrepancies between the observed and optimized parameters may be due to compensating errors due to inadequacies of the model physics and prescribed parameters. Additionally, there are uncertainties in precipitation and other related forcing data, all of which are assumed to be without error. When a long time series of soil moisture is used, as in this study, the surface is a reflectance of the deep soil moisture through capillary redistribution. It was also observed that when optimized parameters from the surface-only retrieval were used, the soil moisture RMSEs were almost equivalent to the results obtained from benchmarking. Additionally, Bandara et al. (2013b) investigated the requirements for the soil hydraulic parameter retrieval of a heterogeneous column of soil, using near-surface soil moisture observations only, and found that the minimum required period was 12 months. With the present work focusing on three years the confidence in the retrieved parameters for the root zone is quite high.

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