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Towards soil hydraulic parameter retrieval from Land Surface Models using near-surface soil moisture data

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Abstract: The water and energy fluxes at the land-atmosphere interface depend heavily on the soil moisture content, which imposes a significant control on evaporation, infiltration and runoff. Nonetheless, temporal soil moisture evolution is not easy to measure or monitor at large scales due to its spatial variability, which is largely driven by the local variation in soil properties and the vegetation cover. As a consequence, soil moisture dynamics are generally estimated using land surface models, with model physics based on low-resolution soil property maps, which may include significant errors due to their underpinning information and spatial scale. Consequently, there is a need for more accurate and detailed soil parameter data sets than are currently available in order for the model to perform reliably.

There are a large number of land surface models with a range of characteristics and model physics. This paper presents an assessment of the soil hydraulic parameter retrieval capability from calibration to surface soil moisture observations using two prominent land surface models, the Community Atmosphere Biosphere Land Exchange (CABLE) model and the Joint UK Land Exchange Simulator (JULES). A synthetic twin experiment was used to achieve the objective of identifying the most suitable of these land surface models to be used in soil hydraulic parameter retrieval using near-surface soil moisture data. This study was conducted in three steps: (a) identifying the soil parameters to which the soil moisture shows the greater sensitivity, (b) assessing the capability of the land surface model to allow the retrieval of identified parameters, and (c) assessing the ability of the model to simulate real conditions.

A range of sensitivity studies were performed for both the CABLE and JULES land surface models using the parameter sensitivity index (S) to identify the model parameters with the highest impact on soil moisture prediction. Having identified the key parameters, a set of assumed ‘true’ parameter values were prescribed for calculating ‘true’ soil moisture dynamics. Those parameters found most sensitive to surface soil moisture observations were then changed to 'best guess’ values, and subsequently retrieved by optimizing the surface soil moisture predictions against those from the 'truth run' using the Parameter ESTimation (PEST) software. Parameter retrieval capability was assessed for both land surface models based on comparison with the ‘true’ soil parameters and deeper layer soil moisture.

Compared to field observation data, both models captured the wetting and drying trends of the real-world scenario, but over-estimated the soil moisture after wet-up periods and under-estimated the moisture for deeper layers. However, JULES showed greater sensitivity to changes in the soil hydraulic parameters when compared to CABLE. Moreover, an unrealistic value for the volume of water at wilting point, in the form of the observed lowest soil moisture, had to be used as an input parameter for CABLE to simulate sensible soil moisture. It is also important to note that in contrast to CABLE, JULES has been formulated to allow depth varying soil parameter data to be assigned to different soil layers with the added flexibility of allowing the user to vary the number of soil layers and their depths. It was therefore concluded that the JULES model is better suited for the long-term work of retrieving soil hydraulic parameters from surface soil moisture observations.

Keywords: *Soil hydraulic parameters, land surface models, JULES, CABLE, PEST*

1. INTRODUCTION

The water and energy fluxes at the land-atmosphere interface depend heavily on the soil moisture content, which imposes a significant control on evaporation, infiltration and runoff. Moreover, the rate of water uptake by vegetation in the vadose zone is regulated by the soil moisture content since soil, besides providing nutrients for plant growth, serves as a reserve for the moisture that plants require. Soil moisture plays an essential role in most scientific disciplines related to environmental sciences. However, the problem is that soil moisture evolution is not easy to monitor on large scales, and although remote sensing techniques have been shown useful in soil moisture detection with passive microwave observations at L-band (Paloscia et al., 1993), there is still a great reliance on the prediction of soil moisture evolution using land surface models.

Land surface models are used to provide a boundary condition to climate models, representing the interactions between the land surface and the atmosphere. Consequently the land surface model must predict the radiation, water, heat and carbon exchanges, with explicit representation of vegetation and soil types. These models generally require meteorological forcing data and parameters of vegetation and soil characteristics as inputs (Abramowitz et al., 2007). Paloscia et al. (1993) describe the two modeling approaches that can be used in estimating the water balance of the Earth's surface as; i) precise yet complex models and ii) simple but crude models. However, both approaches require accurate soil hydraulic parameter information that is spatially representative. The most straightforward method of obtaining soil hydraulic parameters is in-situ measurements, but because of their time consuming nature and the expenses involved, pedotransfer functions are mostly used (Wösten, 1997; Wösten et al., 2001). Extrapolation over large areas (Vereecken et al., 1989) yields crude estimates of soil hydraulic properties with large standard deviations, the accuracy of which deteriorates with the extent of the extrapolation, and hence the accuracy of the model simulations. Remote sensing techniques, using satellite and airborne sensors which are able to supply a long time series of data over wide areas, offer a novel approach to the estimation of soil hydraulic properties with high spatial resolution. Virtual studies by Montzka et. al (2011) have demonstrated the potential to both correct the model states and estimate soil hydraulic parameters using near-surface soil moisture observations with different temporal resolutions. A significant conclusion from their study was that the 3-day overpass that the Soil Moisture and Ocean Salinity (SMOS) mission provides should be able to correct the biases resulting from erroneous soil hydraulic parameters and thus reduce their uncertainty. This is an important finding as the long-term objective of the study presented here is to retrieve soil hydraulic parameters using the remotely sensed surface soil moisture information from the SMOS mission, by harmonizing model simulations with observed surface soil moisture data.

As a first step, this study focuses on two prominent land surface models used in climate forecasting, the Community Atmosphere Biosphere Land Exchange (CABLE) model (Abramowitz, 2006; Kowalczyk et al., 2006) and the Joint UK Land Environment Simulator (JULES) model (Clark and Harris, 2009; Best et al., 2011; Clark et al., 2011), with the objective of studying the capability of each model to allow the retrieval of the most critical parameters. The intent of this work was to maintain the community version of the models, and hence the original program codes were not modified. Of the many parameters used as inputs in these models, the interest here was on the parameters that defined the soil properties. While it would be ideal to retrieve all soil parameters, this is not practical for several reasons. For example, 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 to identify the parameters to which the soil moisture simulation showed the most sensitivity.

2. MODEL DESCRIPTION

2.1. Joint UK Land Environment Simulator – JULES

The Joint UK Land Environment Simulator is a multi-layered model with the capability of simulating the soil moisture and soil temperature at time steps of 30 or 60 minutes. JULES consists of four sub-models, soil, snow, vegetation and radiation. Of these, the focus in this paper is on the soil sub-model and the simulation of soil moisture. By default, JULES is run with four soil layers of 0.10 m, 0.25 m, 0.65 m and 2.0 m thickness, totaling to an overall depth of 3.0 m. However, both the number of layers and their thickness can be varied by the user; the parameters and initial conditions for each of the specified soil layers also need to be specified. Although the Richard's equation is used in the calculation of soil moisture, there is a choice of using either of two commonly used constitutive relationships; Brooks and Corey (1964) or van Genuchten (1980). Dharssi et al. (2009) have shown that, with suitable parameter values, both relationships yield similar results for the soil moisture retention curve over most of the soil moisture range, but that the relationship between the hydraulic conductivity and the soil moisture are different. Hence, throughout the following work, the Brooks and Corey relationship has been used as its parameters can be related to the Clapp and Hornberger parameters required by CABLE. To conform to the CABLE model, the number of layers in JULES was set to six with the depths identical to CABLE. Additional information about the model and its' physics can be found in Clark and Harris (2009), Best et al. (2011), and Clark et al. (2011).

2.2. Community Atmosphere Biosphere Land Exchange – CABLE

The Community Atmosphere Biosphere Land Exchange model is a multi-layered land surface model which simulates the soil moisture and soil temperature for six fixed layers of 0.022 m, 0.058 m, 0.154 m, 0.409 m, 1.085 m and 2.872 m in thicknesses, totaling to an overall depth of 4.6 m. The community version of the model does not make provisions for the user to change either the number of layers or their thickness. Moreover, this model does not facilitate the specification of parameter data for individual layers of the profile. However, it is possible to initialize the soil moisture of all six soil layers. CABLE comprises of five sub-models, namely the radiation model, canopy meteorology model, surface flux model, soil and snow model, and ecosystem respiration model. The focus is again on the soil (and snow) sub-model, which includes three prognostic variables, namely; soil temperature, liquid water and ice content. The soil moisture calculations are also made with the Richard's equation, but with the Clapp and Hornberger (1978) constitutive relationship (Abramowitz, 2006; Kowalczyk et al., 2006; Wang et al., 2011). Kowalczyk et al. (2006) discusses the model physics in detail.

2.3. Parameter ESTimation – PEST

The Parameter ESTimation software (Doherty, 2005) has been used here for retrieval of the soil hydraulic parameters by calibrating the predicted to observed near-surface soil moisture time series. As a nonlinear parameter estimator, PEST can be run independently of any model and easily implemented to estimate parameters, with its automatic calibration procedure minimizing an objective function related to the square difference between the 'observed' and simulated variables. PEST uses the Gauss-Marquardt-Lavenberg algorithm - a method that requires a continuous relationship to exist between model parameters and model outputs, so that it can normally find the local minimum in the objective function in fewer model runs than any other parameter simulation method. The optimal parameter set is defined as that for which the sum of squared deviations between the model-generated observations and experimental observations is reduced to a minimum. For this work, the optimization code was used as is without any modifications. Doherty (2005) discusses the model and its performance in detail.

3. NUMERICAL EXPERIMENTS

A synthetic-twin experimental approach was applied in this study. The predicted soil moisture for a selected soil type and its parameters (kept constant for both models) was used to simulate what is termed a 'true' time series of soil moisture states using the 'true' soil hydraulic parameters. The soil hydraulic parameters belonging to a different soil type were then substituted and the simulated soil moisture states termed 'open loop'. The 'true' twelve-month time series soil moisture data corresponding to the surface layer (0-2.2 cm) was then used to build the objective function that would be minimized by PEST to retrieve the original set of 'true' parameters. The optimized parameter values will have the prefix 'retrieved' throughout the paper.

3.1. Data Sets

This study is for a one-dimensional synthetic soil column. The meteorological forcing data along with the soil and vegetation parameters were obtained from site Y3 of the OzNet (http://www.oznet.org.au/) monitoring network (Smith et al., In review), meaning that a comparison with actual observed soil moisture records could also be undertaken. This particular point is located near Yanco, NSW, with meteorological data also available at 30-minute intervals. When specifying initial conditions for the models, field observation data for soil moisture and temperature corresponding to this station have been used. All data are for the year 2003, which had a record of soil moisture ranging from extremely dry conditions to extremely wet conditions. Figure 1 shows the 12-month field observation of soil moisture for Y3 at three depths.

Since actual soil hydraulic parameters for the simulated depths were not available for Y3 at the time of this work, the models were run using the default Food and Agriculture Organization of the United Nations' (FAO) soil texture map together with the default soil hydraulic parameter interpretation from Rawls et al. (1982). The results corresponded to medium-fine silty clay soil type, and this was used in the 'true' run. For the 'open loop', soil hydraulic properties for a coarse-medium-fine sandy clay loam soil type were chosen, based on the

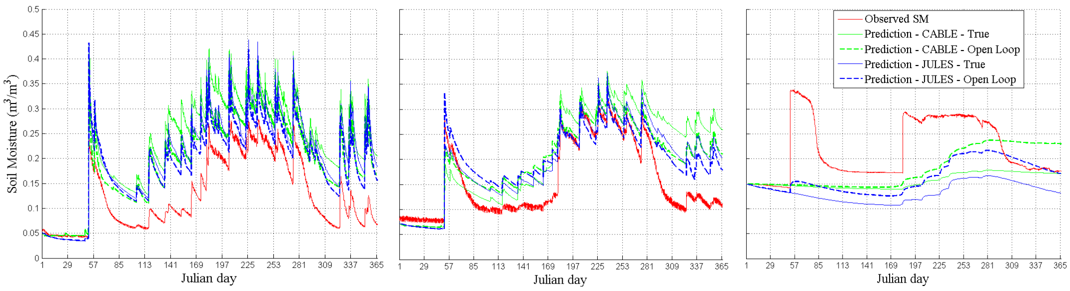

Figure 1. The observed and model simulated soil moisture values, from left to right, a) 0-7cm, b) 0-30cm and c) 30-60cm.

same databases as the 'true' run. To calculate the dry thermal conductivity and heat capacity parameters from soil texture, which are required inputs for the JULES model, equations from Jones (1996) were used.

3.2. Sensitivity Studies

Both models simulate soil temperature as well as soil moisture. For their respective soil modules, CABLE requires eleven soil parameters while JULES uses eight. However, not all of these parameters contribute equally towards soil moisture calculation, and so to identify the parameters that are more sensitive to soil moisture simulation, the parameter sensitivity index has been used. The sensitivity index represents a relative normalized change in output to a normalized change in input. The greater the absolute value of the index, the greater the impact an input parameter has on a particular output (Nearing et al., 1990; Al-Abed and Whiteley, 2002). The sensitivity index (S) is defined as

$$S = \left(\frac{O_2 - O_1}{I_2 - I_1}\right) \frac{I_{avg}}{O_{avg}}, \tag{1}$$

where I_1 and I_2 are the smallest and greatest input values, respectively, tested for a given parameter, I_{avg} is the average of I_1 and I_2, O_1 and O_2 are the model output values corresponding to I_1 and I_2 and O_{avg} is the average of O_1 and O_2. Consequently, for implementation this index is calculated for each model time step.

Three soil moisture time series corresponding to the parameter minus standard deviation, the parameter value itself and the parameter plus standard deviation were used for the values of O_1, O_{avg} and O_2 respectively. As a result, the parameter sensitivity index was a time series with a single value of S calculated at each instant of time. Consequently, the sensitivity index reported for the top layer in Table 1 is the average of the absolute values over the time series. The standard deviations given in Clapp and Hornberger (1978) were used in perturbing the soil parameters. Table 1 contains the parameters that showed the highest sensitivity to soil moisture simulation together with the soil properties and standard deviations (S.D) used to calculate the parameter sensitivity index.

In the sensitivity analysis, the volume of water at wilting point in Rawls et al. (1982) was initially used. However, the resultant soil moisture prediction from CABLE was unrealistic, as the model did not dry-down below the wilting point, and showed a loss of sensitivity to the soil hydraulic parameters. Hence, a value near to the lowest observed soil moisture was used as the volume of water at wilting point for CABLE, resulting in a more realistic soil moisture simulation with higher model sensitivity (Figure 1). While JULES had no such operational limitation, the same wilting point parameter value was used in the work throughout this paper in order to make both models as identical as possible for an unbiased evaluation.

3.3. Parameter Retrieval

To study the parameter retrieval capability of the two models, several parameter combinations were examined, such as the retrieval of a single parameter, retrieval of a subset of parameters, and the retrieval of all parameters sensitive to soil moisture simulations. The number of layers and their thickness have been kept consistent for both models, with six layers of thicknesses 0.022 m, 0.058 m, 0.154 m, 0.409 m, 1.085 m and 2.872 m, thus complying with pre-defined layers of CABLE.

After recording the model simulation corresponding to the 'true' parameters, the soil parameter values were changed to the coarse-medium-fine sandy clay loam soil type, in order to represent the uncertainty in published soil hydraulic parameter maps. It was then attempted to "retrieve" the original parameters using the PEST model, which changes the user specified parameters until a minimum value for the objective function between the 'true' and 'open loop' predictions of surface soil moisture is achieved. Hence, assuming that the top layer at 0.022 m thickness represented the near-surface soil moisture observation from satellite, the model simulations for the top layer were used in the retrieval process.

4. RESULTS AND DISCUSSION

From the sensitivity analysis, six of the eleven soil parameters used in CABLE were found to have a significant influence on soil moisture prediction. Moreover, of the eight parameters that JULES uses, the same six parameters showed the highest sensitivity (Table 1).

The experimental approach included i) retrieval of one parameter at a time, ii) different combinations of two and three parameters, and iii) all six parameters simultaneously. It was observed that the RMSE values of predicted soil moisture were very much lower when a single parameter value is retrieved, as compared to retrieving two or more parameters. However, not all of these parameter retrievals are shown here. Tables 2 and 3, corresponding to the CABLE and JULES models respectively, show an example of the behavior of the soil moisture simulation when three input parameters are presumed to be poorly known. The 'true', 'open loop' and 'retrieved' parameter values are given together with the root mean square error (RMSE) of the simulated soil moisture in the tables. It is observed from Tables 2 and 3 that CABLE yields a lower RMSE in predicted soil moisture using the retrieved parameters when compared to the JULES model, but that the correct parameter values are not as accurately retrieved. It is also observed that the RMSE for the deepest layer is nearly zero for both models, which is mostly because the changes seen in the surface layer are not reflected in the deep layer on the timescales of this simulation.

Soil moisture values predicted by JULES and CABLE corresponding to the parameters used for the 'true' and the 'open loop' runs, plotted against the field observation data for the same dates for depths of 0-0.07 m, 0-0.30 m and 0.30-0.60 m, are shown in Figure 1. Since the simulations have different depths from field observations, all simulated values were brought to the observation depths by using weighted averages. It is observed from the figures that both models over-estimated the soil moisture after a rainfall event and did not dry down as quickly as the field observations. The depth 0.30-0.60 m shows an opposite result, where both models have under-estimated the soil moisture. However, it must be highlighted that the parameters used as inputs for the models have not been calibrated against field data. Some important characteristics and behavioral patterns of the selected land surface models are also summarized in Table 4.

5. CONCLUSION

It was observed that when retrieving two or more parameters simultaneously, an overall low RMSE can be obtained for the surface soil moisture, but not all of the retrieved parameters resemble the 'true' values (not shown here). The possibility to retrieve three parameters simultaneously (shown in Tables 2 and 3) with approximate standard deviations of 0.05 m^3/m^3, 0.08 m^3/m^3 and 0.00001 m^3/m^3 for parameter 'b', suction at saturation and hydraulic conductivity at saturation, respectively, for the JULES model was approximated by PEST. The standard deviations for the 'retrieved' parameters for CABLE, again observed by PEST, were 0.194 m^3/m^3, 0.183 m^3/m^3 and $1.003*10^{-7}$ m^3/m^3 respectively. Some parameters like the parameter 'b' and volume of water at field capacity were better ‘retrieved’ when compared to the other parameters. However, some of these limitations may be due to the selected optimization software and this will be investigated further by assessing the limitations and advantages of different optimization methodologies.

The major disadvantages (shown in Table 4) that can be identified with the CABLE model as compared to JULES is not having an option for multi-layer soil property input data, not having provisions to vary the soil layer thicknesses as desired by the user, and its inability to provide realistic simulations when using a realistic wilting point value. It is therefore concluded that the Joint UK Land Environment Simulator (JULES) is the more suitable land surface model for soil hydraulic parameter retrieval of the two tested here, and will consequently be used in future work on this topic.

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Table 1. Parameter values used together with published uncertainty according to soil type, together with sensitivity index (S). A higher value means the parameter is more sensitive.

Parameter	Value	S.D	S CABLE	S JULES
Parameter 'b' (-)	10.4	4.45	0.196	0.284
Suction at saturation (m)	0.490	0.31	0.048	0.042
Hydraulic conductivity at saturation (mm/s)	0.001	0.0005	0.044	0.108
Volume of water at saturation (m^3/m^3)	0.482	0.064	0.486	0.611
Volume of water at field capacity (m^3/m^3)	0.370	0.064	0.352	0.861
Volume of water at wilting point (m^3/m^3)	0.283	0.064	0.020	0.099

Table 4. Summary of the characteristics of the two models for soil parameter estimation.

Description	JULES	CABLE
Ability to specify multi-layer input data	●	
Ability to enter multi-layer initial conditions	●	●
Ability to retrieve near-perfect parameter values	●	
Ability to match the wetting-drying 'trend' of observations	●[1]	●[1]
Flexibility in varying the depths of the soil layers	●	
Flexibility in varying the number of soil layers	●	

[1] using default parameters from global datasets

Table 2. The "True", "Open Loop" and "Retrieved" parameter values with the root mean square error (RMSE) of soil moisture for each layer of the CABLE model after parameter retrieval and for the open loop. The "True" values of Layer 1 were used as the observations in the retrieval process.

Parameter	"True" Value	"Open Loop" Value	"Retrieved" Value	RMSE ("True"- "Retrieved") (m^3/m^3) Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6	RMSE ("True"- "Open Loop") (m^3/m^3) Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6
Parameter 'b'	10.4	7.12	10.91	0.003	0.003	0.008	0.004	0.005	0.000	0.039	0.030	0.051	0.021	0.017	0.007
Suction at saturation (m)	-0.490	-0.299	-0.200												
Hydraulic conductivity at saturation (mm/s)	0.001	0.006	0.47E-05												

Table 3. As for Table 3 but for the JULES model.

Parameter	"True" Value	"Open Loop" Value	"Retrieved" Value	RMSE ("True"- "Retrieved") (m^3/m^3) Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6	RMSE ("True"- "Open Loop") (m^3/m^3) Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6
Parameter 'b'	10.4	7.12	10.72	0.013	0.016	0.024	0.013	0.004	0.000	0.044	0.028	0.032	0.043	0.038	0.002
Suction at saturation (m)	-0.490	-0.299	-0.457												
Hydraulic conductivity at saturation (mm/s)	0.001	0.006	0.0006												

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