QUANTIFICATION OF THE MODEL PARAMETER UNCERTAINTIES ON SOIL MOISTURE SIMULATION

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ABSTRACT: Knowledge of the unsaturated soil hydraulic properties is mandatory for describing and predicting water flow in the vadose zone. Various types of pedotransfer functions (PTFs) were developed for estimating related parameters in the van Genuchten-Mualem (VGM) model. Unfortunately, no good method currently exists to decide which PTFs should be used for a specific site or application. So this study aims to determine the uncertainty in soil hydraulic parameters on soil moisture prediction. A sensitivity analysis was carried out at three sites (Miyun, Daxing and Guantao) in Hai River Basin, which represent three different underlying surfaces and provide in-situ meteorological and soil moisture measurements. A vertical one dimensional Rechards' equation based on the finite difference method was used, forced with ground-measured rainfall and evapotranspiration data. Compared to the observed soil moisture, the model performance was found to be good, with root mean square error (RMSE) of 0.0313, 0.0359 and 0.0409 for Miyun, Daxing and Guantao, respectively. Secondly, Gaussian error propagation (GEP) principles was used to quantify the random uncertainty of the five parameters (K_s, θ_s , θ_r , α , n) of the VGM model in the surface, root zone and bottom layer on soil moisture simulation. The result shows that the saturated soil moisture (θ_s) and shape parameter (n) in each layer are the most sensitive parameters, only slightly different degree of sensitivity at different sites. Additionally, the response of the entire soil profile moisture to the changes of the most sensitive parameter in each layer was analyzed, which provides a reliable basis to optimize the parameters, and improve the prediction accuracy of the model.

1. INTRODUCTION

Soil moisture dynamics is the central part and the contact link of the Soil-Plant-Atmosphere Continuum system (SPAC), as it's comprehensive response to climate, soil, ecological and other processes in soil water balance. Soil water transport in the vadose zone is considered as the most important and most complex part in hydrological cycle. The Richards' equation (Richards, 1931) is the most general method to compute soil moistures and hydrological fluxes, such as infiltration, infiltration excess, evapotranspiration (ET) and groundwater recharge. Commonly encountered field conditions, such as soil layering, shallow groundwater table and the effect of soil moisture on infiltration, are easily incorporated into Richards' equation (Downer and Ogden, 2004). Soil hydraulic properties (i.e. soil water retention curve and soilhydraulic conductivity) is a fundamental part of solving the Richards ' equation and therefore their accurate determination is essential to model soil moisture dynamics. Unfortunately, investigations for the hydraulic characterization of soils are time-consuming and costly, and the accuracy of the results obtained by the different pedotransfer functions (PTFs) is still debated, in spite of their wide application. Therefore, we may wonder how the uncertainty in soil hydraulic parameters relates to the uncertainty of simulated soil moisture. The incorporation of uncertainty is not a standard practice in hydrologic modeling and there is a lack of framework for assessing parameter uncertainty and propagating the uncertainty through the model.

At present, much work has focused on identifying the uncertainty of the soil hydraulic properties or evaluating the applicability and accuracy of various PTFs. W östen et al. (2001) reviewed the current status of PTFs development, their uncertainty and their practical use in modeling. They showed that quantification of uncertainty in PTFs was useful and that functional evaluation of PTFs was a good tool to assess the desired accuracy of the PTFs for a specific application. Nemes et al. (2006a) tested various PTFs with SWAP and analyzed their performance from multiple aspects. They underlined the importance of the choice of the PTFs to be adopted. Stumpp et al. (2009) evaluated two types of PTFs (ROSETTA and SOILPROP) for their accuracy and applicability by direct evaluation and functional evaluation based on Hydrus-1D.

To date, very few studies have been attempted to investigate the influence of randomness in each parameter of the soil hydraulic properties on the variance of the soil moisture simulation. Coppola et al. (2009) investigated the relative importance of each uncertain and spatially variable parameter that entered the bimodal hydraulic functions in the flow processes studied based on Monte Carlo analysis. They argued that the contribution of each parameter depended only partly on the coefficient of variation, much more on the sensitivity of the model to the parameters and on the flow process being observed. Möders (2005) applied Gaussian error propagation (GEP) to calculate plant- and

soil-parameter-caused uncertainty of surface fluxes predicted by the hydro-thermodynamic soil-vegetation scheme. In this study, GEP principles was applied at three sites (Miyun, Daxing and Guantao) in Hai River Basin, to quantify the influence of the random uncertainty of the parameters in the VGM model on the soil moisture obtained by a one-dimensional Richards' equation on the basis of the finite difference method. Assessing the weight that each parameter has in a specific flow process allows us to focus our investigation on those parameters which dominate systemuncertainties. This is the first step to better understanding the effect of these uncertainties on model prediction.

2. MATERIALS AND METHODS

2.1 Governing equations

Combination of Darcy's law and the principle of mass conservation leads to the well-known Richards' equation. In the vertical dimension, the θ -based Richards equation can be expressed as,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta) \frac{\partial \theta}{\partial z} \right] - \frac{\partial K(\theta)}{\partial z} - S$$
⁽¹⁾

Where θ is volumetric soil moisture content (cm³cm⁻³), t is time (min), z is the elevation relative to a plane (positive downward) (cm), K(θ) is unsaturated hydraulic conductivity (cm/min), D(θ) is soil diffusivity (cm²/min), and S is soil moisture sink term (e.g., transpiration loss in the rooting zone), which was not included in the original equation. The soil hydraulic properties were parameterized using the Van Genuchten–Mualem constitutive relationships (Mualem, 1976; Van Genuchten, 1980):

$$S_{e} = \frac{\theta - \theta_{r}}{\theta_{r} - \theta_{r}} = \left[\left(1 + |\alpha h| \right)^{n} \right]^{\frac{1}{n}}$$
⁽²⁾

$$K(\theta) = K_{s} S_{e}^{0.5} \left[1 - \left(1 - S_{e}^{\frac{n}{n-1}} \right)^{\frac{n-1}{n}} \right]^{2}$$
(3)

$$D(\theta) = \frac{K_s S_e^{\left(0.5 - \frac{n}{n-1}\right)}}{\alpha(n-1)(\theta_s - \theta_r)} \left[(1 - S_e^{\frac{n}{n-1}})^{\frac{n-1}{n}} + (1 - S_e^{\frac{n}{n-1}})^{\frac{1-n}{n}} - 2 \right]$$
(4)

Where, S_e is degree of saturation (cm³cm⁻³), θ_s is the saturated moisture content (cm³cm⁻³), θ_r is the residual moisture content (cm³cm⁻³), K_s is the saturated hydraulic conductivity (cm/min), α is related to the inverse of air entry parameter which is the inverse of capillary fringe thickness (cm⁻¹), and n is the shape parameter or pore size distribution parameter.

Running the model required specifying the hydraulic parameters θ_s , θ_r , α , n and Ks. These parameters were estimated using ROSEITA (Schaap et al., 2001), a pedotransfer function model that predicts hydraulic parameters from soil texture and related data. Rosetta contains a hierarchy of pedotransfer functions that can be used depending upon available data. We predicted the hydraulic parameters using ground-measured data, including bulk density and percentages of sand, silt, and clay (Table 1). According to the measured soil mechanical composition data, the soil profile was modeled as a three-layer system (surface, root zone and bottom) with differing soil hydraulic properties.

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	Table 1	Measured soil textural and bulk density data, along with estimated hydraulic parameters by						y Rosetta.	
	Clay	Silt	Sand	bulk density	$ heta_{ m r}$	$\theta_{ m s}$	а	n	Ks
	(<2um)	(2-50.um)	(50-2,000um)	(g/cm3)	(cm3cm-3)	(cm3cm-3)	(cm-1)		(cm/min)
GT									
0-25	41.68%	54.84%	3.48%	1.47	0.0933	0.4569	0.0107	1.4098	0.003465
26-45	56.64%	40.35%	3.01%	1.47	0.0982	0.4658	0.0151	1.2921	0.003403
45-100	30.09%	47.76%	22.15%	1.53	0.0768	0.4026	0.0089	1.4808	0.003431
MY									
0-15	23.63%	53.22%	23.15%	1.38	0.0724	0.4211	0.0064	1.6028	0.009563
16-50	23.84%	48.89%	27.27%	1.48	0.0687	0.3958	0.0075	1.5501	0.005472
50-100	15.95%	35.32%	48.73%	1.49	0.0511	0.3772	0.0145	1.457	0.011306
DX									
0-30	17.24%	58.73%	24.03%	1.40	0.0619	0.3991	0.0054	1.6566	0.012965
30-50	18.32%	55.92%	25.77%	1.49	0.0603	0.3801	0.0063	1.6048	0.007653
50-100	17.86%	58.23%	23.91%	1.40	0.0629	0.4007	0.0055	1.6528	0.012382

Eq. (1) is subjected to specified initial and boundary conditions. The initial condition was implemented using cubic spline interpolation based on the soil moisture of the observation depths to obtain the soil moisture in soil profile. For the field case, the top boundary is governed by the atmospheric conditions, whose processes might be infiltration due to rainfall/irrigation or evaporation. While a free drainage condition (unit hydraulic gradient) or constant moisture content was used at the bottom, which is appropriate due to fact that the water table was far below the root zone.

$$D(\theta_0) \frac{\partial \theta}{\partial z}\Big|_{z=0} + K \ (\theta_0) = P(t) - E(t)$$
(5)

$$\left. \frac{\partial \theta}{\partial z} \right|_{z=l} = 0 \quad \text{or } \theta_l(t) = \theta_l(0) \tag{6}$$

Analytical solution of this non-linear partial differential equation described by Richards for the field conditions is not available. Hence, one has to discretize the equation into space and time using either finite difference or finite element methods. Finite elements are advantageous at an irregular geometry in 2 and 3-dimensional flow domains. In one dimension finite difference is advantageous because it needs no mass lumping to prevent oscillations (Van Genuchten, 1982; Pan et al., 1996), and is relatively easy to conceive and to implement in numerical routines. A model based on the fully implicit backward finite difference scheme has been developed in the IDL language to solve the equation numerically.

An essential element of the numerical solution of Richards's equation is that the solution converges as the spatial resolution increases. Using a sufficiently fine discretization near the soil surface is critical, using fine discretization deep in the soil column achieves little benefit (Downer and Ogden, 2004). In this study, 100cm of the soil profile was discretized into 53 nodes, The cell size in the top layer (0-40cm) was 1 cm and cell size in the bottom layer(40-100cm) was 5 cm, which greatly improved the operation speed while ensure the prediction accuracy of the model.

The convergence criterion below was implemented in the iterative solution of RE.

$$\max\left|\frac{\theta_{i}^{j+l(p)} - \theta_{i}^{j+l(p-1)}}{\theta_{i}^{j+l(p-1)}}\right| \le e$$
(7)

Where *e* is absolute water content tolerance for nodes (its recommended value is 0.0001). This parameter represents the maximum desired absolute change in the value of the water content between two successive iterations during a particular time step. Subscript i represents each node on the soil profile, Superscript j+1 denotes the next time, P indicates the number of iterations. The variable, optimal time step should minimize the computational effort of a simulation. The number of iterations needed to reach convergence in the former time step, N_{it}, can be effectively used to derive the optimal time step according to the following criteria.

 N_{it} <3: multiply time step with a factor 1.3;

 $3 \leq N_{it} \leq 6$: keep time step the same;

 N_{it} >6: divide time step by a factor 1.3.

The actual time step was determined using above criteria in combination with an initial time step, specified minimum and maximum time steps.

2.2 GAUSSIAN ERROR PROPAGATION (GEP) PRINCIPLES

The soil moisture simulated by the model is a function of $\phi = f(x_1, \dots, x_n)$ of one or more empirical parameters x_i that are the mean values obtained from measurements or simulated by other experience functions. The simulated soil moisture will be "error" burdened by an amount σ_{ϕ} resulting from the random variability of empirical parameters

usually characterized by standard deviations σ_{x_i} . GEP principles (e.g., Kreyszig 1970; Meyer 1975) permit determining a predicted flux's statistical uncertainty. The standard deviation of the predicted flux was obtained by the error propagation formula:

$$\sigma_{\phi} = \sqrt{\sum_{i=1}^{n} \left(\frac{\partial \phi}{\partial x_{i}}\right)^{2} \sigma_{x_{i}}^{2} + 2\sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial \phi}{\partial x_{i}} \frac{\partial \phi}{\partial x_{j}} \sigma_{ij}}$$
$$= \sqrt{\sum_{i=1}^{n} \left(\frac{\partial \phi}{\partial x_{i}}\right)^{2} \sigma_{x_{i}}^{2} + 2\sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial \phi}{\partial x_{i}} \frac{\partial \phi}{\partial x_{j}} \rho_{ij} \sigma_{x_{i}} \sigma_{x_{j}}}}$$
(8)

Where ρ_{ij} is the correlation coefficient between two different parameters X_i and X_j . In this study assuming it is independent between the input parameters, $\rho_{ij}=0$, then the simplified form of the above formula can be written as:

$$\sigma_{\phi} = \sqrt{\sum_{i=1}^{n} \left(\frac{\partial \phi}{\partial x_{i}}\right)^{2}} \sigma_{x_{i}}^{2} = \sqrt{\sum_{i=1}^{n} \left\{\phi, \sigma_{x_{i}}\right\}^{2}}$$
(9)

Here n represents the number of empirical parameters. $\sigma_{x_i}^2$ the variances, $\{\phi, \sigma_{xi}\}$ and σ_{ϕ} are denoted contribution

term of the *i*th parameter and the total error of the output respectively. Equation (9) assumes that 1) errors are normal distributed and 2) errors are independent between various model parameters, which is justified for these parameters.

2.3 Experimental design

The above model was implemented by IDL language and conducted at three sites in Hai River Basin: Miyun

(40°37′50.82″N, 117°19′23.83″E, MY) from 23th April to 30th June in 2009, Daxing (39°37′16.7″N, 116°25′37.2″E, DX) from 21th August to 30th September in 2009, Guantao (36°30′54.1″N, 115°07′38.7″E, GT) from 16th June to 16th August in 2008. Broader distribution of three stations represent three typical underlying surface types in Hai River Basin: northern mountains (fruit trees, maize / bare ground), central suburban farmland (wheat / corn, vegetables, fruits) and farmland in southern plains (winter wheat / maize, cotton). Eddy-covariance system (EC), large aperture scintillometer (LAS) and automatic weather stations were installed in three sites. Soil moisture sensors (Decagon: ECH2O-10) were installed in the profile at depths of 2 (only in Guantao), 5, 10, 20, 40, 60 and 100cm, respectively.

The HYDRUS-1D simulations were also conducted using the same data at three sites, as a model of cross-validation. The root mean squared error (RMSE) between simulated (θ_i) and observed values ($\hat{\theta}_i$) was calculated to evaluate the performance of the model.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\theta_i - \hat{\theta}_i)^2}$$
(10)

On the assumption that systematic errors have been excluded, the GEP analysis based on the calculation experiment consists of the following procedures:

- 1. Control experiment: throughout the sensitivity study, the soil moisture was taken as a "true value" simulated by the model based on the soil hydraulic parameters θ_s , θ_r , α , n and Ks taken as the default values in table 1.
- 2. Generate random sample of individual parameter: the mean value was the default parameter value, and standard deviation was set to be 10% of the default parameter value, then normal distribution random samples (n) of the parameter were generated;
- 3. Run a series of simulations: in each simulation the individual parameter values in one case was replaced by the randomsample while all other parameters were held at their baseline values, to get time series of the soil moisture profile;
- 4. Calculate standard deviations of all the output series at every moment at each depth, which were contribution terms of the individual parameter at every moment in the soil profile.
- 5. Repeat (2) (4) for each model parameter, to get the contribution term of each parameter.

$$\sigma_{\phi}^{1} = \{\phi, \sigma \mathbf{x}_{1}\}, \quad \sigma_{\phi}^{2} = \{\phi, \sigma \mathbf{x}_{2}\}, \quad \cdots \quad \sigma_{\phi}^{n} = \{\phi, \sigma \mathbf{x}_{n}\}$$
(11)

6. Apply GEP error propagation formula to calculate the total error as a consequence of the errors in the parameters.

$$\sigma_{\phi} = \sqrt{\left(\sigma_{\phi}^{1}\right)^{2} + \left(\sigma_{\phi}^{2}\right)^{2} + \dots + \left(\sigma_{\phi}^{n}\right)^{2}}$$
(12)

7. The contributions rate of individual parameter accounted for the total error (i.e. the percentage standard deviations (PSD) of the individual parameter in entire standard deviations) was calculated by PSD= $\sigma_{\phi}^{i}/\sigma_{\phi}$.

3. RESULTS AND DISCUSSION

3.1 Performance evaluation

For each site, the soil moisture simulated by the model in this study and hydrus-1D were compared to the in-situ observations. The RMSE of simulated soil moisture corresponding to observed values are showed in Table 2. It indicates that the model with smaller RMSE than the HYDRUS-1D software has a better consistency with the observation. The total RMSE of the model simulated soil moisture in

Table 2 RMSE of simulated soil moisture corresponding to observed values								
	2cm	5 cm	10 cm	20 cm	40 cm	60 cm	100cm	total
Miyun								
simulation		0.0675	0.0317	0.0256	0.0340	0.0254	0.0042	0.0313
HYDRUS		0.0992	0.0654	0.0197	0.0262	0.0106	0.0042	0.0376
Daxing								
simulation		0.0168	0.007	0.0401	0.0797	0.0402	0.0319	0.0359
HYDRUS		0.0428	0.0286	0.0652	0.1208	0.0676	0.0631	0.0647
Guantao								
simulation	0.0509	0.0484	0.0491	0.0291	0.0659	0.0104	0.0330	0.0409
HYDRUS	0.0728	0.0689	0.0692	0.0259	0.0385	0.0212	0.0304	0.0467

Miyun, Daxing and Guantao are 0.0313, 0.0359 and 0.0409, respectively, while the HYDRUS-1D software are 0.0376, 0.0647 and 0.0467, respectively. Simulated soil moisture has a good agreement with observed soil moisture, and model simulation results are better than the results of HYDRUS-1D software. Hence, the model we used here is reliable enough to simulate the soil water dynamic changes at each depth of soil profile, and the sensitivity analysis of the model can be carried out.

3.2 Uncertainty and sensitivity assessment

In order to identify critical parameters, we estimate the mean contribution of individual parameter to the whole soil profile whose contribution to the uncertainty has been time-averaged according to its own time series (see Table 3). The effects of the uncertainty in the parameters on the predicted soil moisture can vary strongly. Figure. 1 show that at

three sites, the contributions rate of the saturated soil moisture (θ_s) and shape parameter (n) in each layer all exceed other terms by more than an order of magnitude, which indicate θ_s and n are critical parameters and more sensitive than other parameters. However, there is slightly different degree of sensitivity at different sites. In Guantao and Miyun, the total errors are 0.03211 and 0.01551, respectively. The contributions rates of θ_s and n in each layer induced soil moisture uncertainty are of a similar order of magnitude. In Daxing, the total error is 0.02134, and the contributions of θ_s and n in the bottom layer are significantly higher than that in surface and root zone layers, which lead to their contribution rates are larger than 50%. We can conclude that the saturated soil moisture (θ_s) and shape parameter (n) are the highest sensitivity to the simulation of soil moisture and the largest contribution rate to the uncertainty of soil moisture. Improving the two parameter precision is expected to improve soil moisture simulation. In fact, this is consistent with some existing research results. Gribb et al. (2009) found that simulations of $\theta(t)$ could be significantly improved by simply replacing the saturated and residual moisture contents with the maximum and minimum measured moisture contents. We further take account of the research result of Baroni et al. (2010) who showed a high variability of the soil hydraulic parameter values in the different sets, especially in case of the saturated hydraulic conductivity Ks and of the parameter α , so we can conclude that the hydraulic parameters with the highest relative error are not necessarily the greatest contributors to the standard deviation of the predicted soil moisture, as Mölders (2005) and Coppola et al. (2009) have found from their research.

Table 3 the contribution of individual parameter in the	ne surface, root zone
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and bottom layer at 3 sites.							
	Ks	θ_{s}	$ heta_{ m r}$	α	n		
GT							
0-25	0.002948	0.01791	0.002559	0.002886	0.007085		
26-45	0.000958	0.009357	0.001173	0.001702	0.011374		
45-100	0.002357	0.012268	0.0018	0.000165	0.009595		
MY							
0-15	0.000159	0.001029	0.000121	0.000232	0.001874		
16-50	0.001214	0.007704	0.000949	0.001039	0.009202		
50-100	0.000739	0.004257	0.000675	0.000656	0.006384		
DX							
0-30	0.0001606	0.000921	7.25E-05	0.00032	0.001028		
30-50	0.000192	0.001139	0.000161	0.000512	0.00176		
50-100	0.0018216	0.014893	0.001431	0.001480	0.014736		

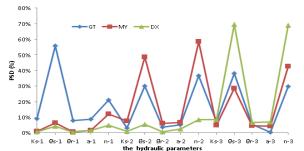


Figure. 1 the contributions rate of individual parameters accounted for the total error at three sites. Parameter suffix -1,-2,-3 stands for the parameter in surface, root zone and bottom layer, respectively.

Additionally, the effect of $\pm 10\%$ perturbations to the critical hydraulic parameters (θ_s and n) at a time in individual soil layers on the simulated soil moisture in soil profile was evaluated. A parameter was changed by ten percent of its value, then the simulation was run and the effects of that parameter change on the soil moisture at each depth were assessed by calculating the mean deviation (*MD*) between the simulated soil moisture(θ_i) from the perturbation parameter and the "true value" ($\hat{\theta}_i$).

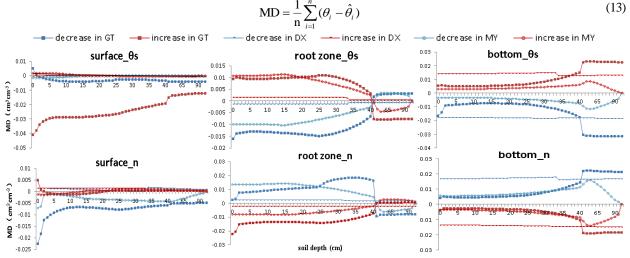


Figure.2 soil moisture changes at each depth in response to perturbations of θ_s and n in each layer in Miyun, Daxing, Guantao sites.

The *MD* at each depth at three sites is showed in Figure.2. Here, a positive (negative) MD of the soil moisture represents an increase (decrease) of the simulated soil moisture due to the changed parameter. It shows that the soil moisture profile respond differently to the change of parameters of each layer. Except for Guantao, the effect of perturbations of θ_s and n in the surface layer on soil moisture is small with no obvious pattern found in their effects on soil moisture profile, which may indicate that other factors like rainfall and evaporation can greatly account for this phenomenon. The impact of θ_s and n change in root zone layer in Daxing is as lo small, while in Miyun and Guantao,

a critical point near the boundary between root zone layer and bottom layer, on the two sides of which the impact of parameter change on the soil moisture is opposite, for the reason that the soil unsaturated hydraulic conductivity and soil diffusivity generally increase with the increase of n, but decrease with the increase of θ_s and vice versa, whose decrease directly impact the drainage of water out of the root zone and leads to the soil moisture increase above the root zone layer, while decrease in the bottom layer. The entire soil moisture profile response to perturbations of θ_s and n in the bottom layer is relatively consistent at three sites that soil moisture generally increase with θ_s , but decrease with the increase of n and vice versa. In sum, the influence of parameter change of θ_s and n in root layer and the bottom layer on soil moisture have a major influence on the entire soil moisture profile simulation, not as simple as in homogeneous soil condition. Unfortunately, in most cases soil was taken as homogeneous, without considering of the vertical heterogeneity.

4. CONCLUSIONS

The soil moisture (θ)-based Richards' equation based on the finite difference method was used to govern the vertical water movement at three sites, and the model performance was found to be good, with root mean square error (RMSE) of 0.0313, 0.0359 and 0.0409 for Miyun, Daxing and Guantao, respectively. Therefore, the model is reliable enough to accurately simulate the soil water dynamic changes at each depth of soil profile.

GEP principles was introduced to examine model uncertainty in predicted soil moisture caused by statistical uncertainty of soil hydraulic parameters (θ_s , θ_r , a, n and Ks) occurring in the Rechards' equation at three sites. Our analysis gave evidence that uncertainty in the saturated soil moisture (θ_s) and shape parameter (n) identified as the critical parameters dominated uncertainty in soil moisture, and that increasing accuracy of the critical parameters would reduce model uncertainties.

The response of the entire soil profile moisture to the changes of the most sensitive parameters was analyzed at 3 sites. We found that the response of soil moisture to the hydraulic parameters was not simply decrease with depth, and that θ_s and n in root layer and the bottom layer have a major influence on the entire soil moisture profile simulation. Therefore we suggest that soil vertical heterogeneity should be considered in soil moisture simulation.

Since GEP method can identify critical parameters, the GEP analysis could form a basis for prioritizing which parameters to determine with higher accuracy aimed at improving soil moisture simulation.

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