Hydrological Sciences Journal
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/thsj20

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Available online: 11 Apr 2012

To cite this article: Feifei Pan, Robert B. McKane & Marc Stieglitz (2012): Identification of optimal soil hydraulic functions and parameters for predicting soil moisture, Hydrological Sciences Journal, 57:4, 723-737

To link to this article: http://dx.doi.org/10.1080/02626667.2012.674642

Identification of optimal soil hydraulic functions and parameters for predicting soil moisture

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Received 8 February 2011; accepted 19 October 2011; open for discussion until 1 November 2012

Editor D. Koutsoyiannis; **Associate editor** D. Hughes

Citation Pan, F., McKane, R.B. and Stieglitz, M., 2012. Identification of optimal soil hydraulic functions and parameters for predicting soil moisture. *Hydrological Sciences Journal*, 57 (4), 723–737.

Abstract The accuracy of six combined methods formed by three commonly-used soil hydraulic functions and two methods to determine soil hydraulic parameters based on a soil hydraulic parameter look-up table and soil pedotransfer functions was examined for simulating soil moisture. A novel data analysis and modelling approach was used that eliminated the effects of evapotranspiration so that specific sources of error among the six combined methods could be identified and quantified. By comparing simulated and observed soil moisture at six sites of the USDA Soil Climate Analysis Network, we identified the optimal soil hydraulic functions and parameters for predicting soil moisture. Through sensitivity tests, we also showed that adjusting only the soil saturated hydraulic conductivity, K_s, is insufficient for representing important effects of macropores on soil hydraulic conductivity. Our analysis illustrates that, in general, soil hydraulic conductivity is less sensitive to K_s than to the soil pore-size distribution parameter.

Key words soil moisture; Richards equation; soil hydraulic functions; soil parameters; macropore; soil pore size distribution index

Identification des fonctions et des paramètres hydrauliques optimaux des sols pour prévoir leur humidité

Résumé Nous avons examiné l'exactitude de six méthodes de simulation de l'humidité du sol, issues de la combinaison de trois fonctions hydrauliques du sol couramment utilisées et de deux méthodes de détermination de paramètres hydrauliques du sol basées sur une table de conversion des paramètres hydrauliques du sol et des fonctions de pédotransfert. Nous avons utilisé une nouvelle approche d'analyse des données et de modélisation qui élimine les effets de l'évapotranspiration, de sorte que les sources spécifiques d'erreur au sein des six méthodes combinées ont pu être identifiées et quantifiées. En comparant l'humidité du sol simulée et observée sur six sites du Réseau d'analyse climatique des sols, nous avons identifié les fonctions et les paramètres hydrauliques optimaux des sols pour prévoir l'humidité du sol. Par des tests de sensibilité, nous avons également montré qu'ajuster seulement la conductivité hydraulique à saturation du sol, K_s, est insuffisant pour représenter les effets importants des macropores sur la conductivité hydraulique du sol. Notre analyse montre, qu'en général, la conductivité hydraulique du sol est moins sensible au K_s qu'au paramètre de distribution de la taille des pores du sol.

Mots clefs humidité du sol; équation de Richards; fonctions hydrauliques du sol; paramètres du sol; macropores; indice de distribution de la taille des pores du sol

1 INTRODUCTION

1.1 Background information

Soil moisture is an important variable influencing the partitioning of solar radiation into sensible and latent heat fluxes and the separation of precipitation into infiltration and surface runoff, and thus plays a vital role in affecting the atmospheric boundary layer, weather and climate (e.g. Deardorff 1978, Dickinson *et al*. 1986, 1993, Cuenca *et al*. 1996).

ISSN 0262-6667 print/ISSN 2150-3435 online

http://dx.doi.org/10.1080/02626667.2012.674642
http://www.tandfonline.com

Accurate estimation of the effects of soil physical properties on soil moisture dynamics is a challenging and longstanding problem in hydrology (e.g. Ek and Cuenca 1994, Shao and Irannejad 1999), mainly because of uncertainties in soil hydraulic parameters and hydraulic functions, particularly the relationship between pressure head (ψ) and water content (θ), and between hydraulic conductivity (K) and water content (θ) (hereafter, the ψ–θ relationship and the K–θ relationship, respectively).

Because it is difficult to quantify ψ–θ and K–θ relationships (Dingman 2002), some empirical relationships have been proposed. The most commonly-used soil ψ–θ and K–θ relationships were suggested by Brooks and Corey (1964) (hereafter referred to as BC), Campbell (1974—CA), and van Genuchten (1980—vG). Both the BC and the CA functions are commonly used in land surface–atmosphere interaction models, such as: the Biosphere–Atmosphere Transfer Scheme (BATS, Dickinson *et al*. 1986, 1993), the Simple Biosphere model (SiB1 and SiB2, Sellers *et al*. 1986 and 1996), the Coupled Atmosphere–Plant Soil model (CAPS, Mahrt and Pan 1984, Pan and Mahrt 1987), the TOPMODEL-based Atmosphere Land Surface Transfer scheme (Famiglietti and Wood 1994, Peters-Lidard *et al*. 1997), the Catchment-based Land Surface model (CLSM, Koster *et al*. 2003), the Variable Infiltration Capacity scheme (VIC, Liang *et al*. 1994, 1996), and the Common Land Model (CLM, Dai *et al*. 2003). Unlike the BC and the CA functions, the vG function is seldom applied in land surface–atmosphere interaction models, although it is commonly-used in soil physical hydrological models, e.g. HYDRUS (Simunek *et al*. 1998). One possible reason is that, to accurately simulate soil moisture dynamics, the soil parameters in the vG function must be calibrated (e.g. Guber *et al*. 2009).

All of the ψ–θ and K–θ relationships mentioned above have a number of parameters that depend on soil texture. For any given application, there are generally two ways to determine the values of these parameters in the BC, CA and vG functions. The first method is to first determine the soil texture, then find the values from a soil hydraulic property table that lists typical values for each soil texture type. The most commonly-used table is that given in Rawls *et al*. (1982—RA), which was based on 1320 soil samples collected from 32 states in the USA (Rawls *et al*. 1982). The second method is to directly calculate values based on empirical relationships, also known as soil pedotransfer functions (PTFs) (Bouma 1989), between these parameters and soil particle-size distribution (PSD) (i.e. sand and clay contents) (e.g. Clapp and Hornberger 1978, Cosby *et al*. 1984, Saxton *et al*. 1986). Because the PTFs of Cosby *et al*. (1984—CO) have fewer parameters than those of Saxton *et al*. (1986—SA), and were developed based on the work of Clapp and Hornberger (1978—CH), CO's PTFs are most commonly used in hydrological models.

1.2 Previous studies

According to the preceding overview, there are at least 12 combined methods that can be used to determine soil ψ–θ and K–θ relationships (see Table 1). Which combination of soil hydraulic functions (BC, CA or vG) and soil hydraulic parameters (look-up tables or PTFs) is best in terms of accuracy of soil moisture predictions? Several studies have focused on this issue. Ek and Cuenca (1994) conducted the first study of this problem, focused on the effects of soil hydraulic functions and soil parameters on modelling surface fluxes and atmospheric boundary layer development. They found that the pore size distribution index b, a scaling exponent in the power functions of soil hydraulic conductivity and pressure head (see Table 3), is the most sensitive soil parameter and has a strong impact on the modelled surface energy balance and atmospheric boundary-layer development (Ek and Cuenca 1994). Since then, there have been several other similar studies, but most of them focused on the effects of ψ–θ and K–θ relationships and soil parameters on water and energy fluxes modelled by a one-dimensional hydrological model (e.g. the Richards equation) coupled with a soil–vegetation–atmosphere transfer (SVAT) scheme. Sun and Bosilovich (1996) investigated the sensitivity of the planetary boundary-layer development to

Table 1 The 12 commonly-used combinations of soil hydraulic functions and parameters.

Soil parameters*	Soil hydraulic functions†		
	BC	CA	vG
RA	BC-RA	CA-RA	vG-RA
CO	BC-CO	CA-CO	vG-CO
CH	BC-CH	CA-CH	vG-CH
SA	BC-SA	CA-SA	vG-SA

* RA (Rawls *et al*. 1982); CO (Cosby *et al*. 1984); CH (Clapp and Hornberger 1978); SA (Saxton *et al*. 1986).
† BC (Brooks and Corey 1964); CA (Campbell *et al*. 1974); vG (van Genucheten 1980).

soil texture. Shao and Irannejad (1999) studied the effect of soil hydraulic functions on soil moisture predictions and associated aspects of land-surface modelling. Other investigators studied four ψ–θ and K–θ relationships, including Brooks and Corey (1964), Clapp and Hornberger (1978), van Genuchten (1980) and Broadbridge and White (1988). Their numerical tests showed that the vG model appeared to perform the best, while the BC and CH models also gave good and consistent results. The BW model did not perform well. Shao and Irannejad (1999) also found that, in contrast to the vG model, the BC and CH models are numerically efficient. Braun and Schädler (2005) showed that the vG /RA model gave the best agreement between observed and simulated soil water contents. Schädler (2007) followed the work of Braun and Schädler (2005), and found that, in terms of root mean square error (RMSE), bias and correlation coefficient, the best results were obtained with the combined functions of CA and CO, vG and CH, and vG and RA.

There is no doubt that soil hydraulic functions and parameters play an important role in modelling water and energy fluxes between the atmosphere and the land surface, and, consequently, affect simulation of the atmospheric boundary-layer development. However, approaches that include a SVAT scheme in the Richards equation can introduce uncertainty in the land-surface parameterization scheme (e.g. Franks *et al*. 1997, Varado *et al*. 2006) and, consequently, in the results determining which combination of functions and parameters is the best in terms of accuracy of the simulated soil moisture. To resolve this issue, in this study we only apply the Richards equation to a single soil column from 10 to 50 cm, without coupling with any SVAT scheme, thereby eliminating the sink terms (i.e. evaporation and transpiration). To eliminate the sink terms in the Richards equation without creating errors in simulated soil moisture, we selected study sites and designed numerical experiments according to the criteria and methodology discussed in Section 2.

1.3 Objectives

The objective of this study is to investigate the effects of different soil hydraulic functions and parameters describing soil ψ–θ and K–θ relationships on the accuracy of soil moisture simulations. Through comparing the simulated and observed soil moisture, we evaluated the following six combinations of commonly-used soil hydraulic functions and soil parameters: BC-RA, BC-CO, CA-RA, CA-CO, vG-RA and vG-CO. In addition to these six combinations, we also evaluated the effects of two other factors, rock content (i.e. particle size > 2 mm) and macropores in soils that can potentially play a role in affecting soil moisture predictions. In particular, because most published soil parameter values and hydraulic relationships were developed based on soil samples from which rocks were removed, we evaluated whether a rock content correction term for soil porosity and saturated hydraulic conductivity can improve soil moisture predictions (Rawls *et al*. 1982). Similarly, because soil macropores (large-diameter conduits in the soil, created by plant roots, soil cracks, soil fauna and microbes) can substantially increase soil hydraulic conductivity, we evaluated a macropore correction term for soil moisture predictions. This paper is organized as follows: Section 2 introduces the study sites and observed soil moisture data; Section 3 describes the methodology; Section 4 presents and discusses simulated soil moisture results in comparison to observed data; and Section 5 is a summary of the major findings.

2 STUDY SITES AND SOIL MOISTURE DATA

The soil moisture data used in this study were collected at sites of the Soil Climate Analysis Network (SCAN), a comprehensive, nationwide soil moisture and climate information system administrated by the US Department of Agriculture Natural Resources Conservation Service (USDA NRCS) through the National Water and Climate Center (NWCC), in cooperation with the NRCS National Soil Survey Center (NSSC) (Seyfried *et al*. 2005, Schaefer *et al*. 2007). The SCAN system measures soil moisture content hourly at 5, 10, 20 and 50 cm. The archived data at each SCAN site are publicly available and were downloaded from http://www.wcc.nrcs.usda.gov/scan.

In this study, the observed soil moisture at 10 and 50 cm collected at the SCAN sites are used as the upper and lower boundary conditions for solving the one-dimensional Richards equation given as follows:

$$\frac{\partial\theta(z,t)}{\partial t} = -\frac{\partial K(\theta,z)}{\partial z} + \frac{\partial}{\partial z}\left[K(\theta,z)\frac{\partial\psi(\theta,z)}{\partial z}\right] \quad (1)$$

where θ is volumetric soil moisture [%V/V], K and ψ are soil hydraulic conductivity [L/T] and pressure head [L], respectively, and z is distance [L] measured vertically downward, e.g. $z = 0$ at the surface. In equation (1), we have omitted both the plant uptake and evaporation (E), or evapotranspiration (ET) terms. As discussed in Section 1, the main reason we dropped the sink terms from the Richards equation is to eliminate errors in the simulated soil moisture due to the uncertainty in the evapotranspiration parameterization scheme. To drop the sink terms in the Richards equation without inducing errors, we selected a sub-set of SCAN sites that satisfy the following conditions:

(i) a continuous soil moisture record during the winter season, specifically December–February;
(ii) an absence of freezing conditions at any time within the soil profile; and
(iii) a bare soil surface (no vegetation).

These conditions ensure that evaporation is negligible, and that any loss of water vapour from evaporation is generally from the top few millimetres, assuming an absence of soil cracks that typically are present only during extremely dry conditions. Therefore, we set the upper boundary for our soil moisture simulations at 10 cm to eliminate errors associated with omitting the E or ET term in the Richards equation.

Based on the considerations described above, six SCAN sites across the southern USA met our site selection criteria. Three sites are in Alabama: AL2053 (34°54′N, 86°32′W), AL2057 (34°47′N, 86°33′W) and AL2113 (34°12′N, 86°48′W); two in Arkansas: AR2030 (34°51′N, 91°53′W) and AR2090 (35°13′N, 92°55′W); and one in Georgia: GA2027 (31°30′N, 83°33′W). The soil texture class and clay, sand and rock contents are listed in Table 2. There are six soil texture classes (i.e. silty clay loam, silty loam, loam, clay loam, clay and sand) between 0–50 cm at these sites, representing about 54% (6/11) of USDA soil texture classes. The land cover type of the six sites is bare ground. Some vegetation may surround some sites, but, at the soil moisture sampling locations, the land surface is free of vegetation.

3 METHODOLOGY

Prior to solving equation (1), we first need to choose ψ–θ and K–θ relationships. In this study, six combinations of soil hydraulic functions and soil parameters (BC-RA, BC-CO, CA-RA, CA-CO, vG-RA and vG-CO) were chosen, as described in Section 1.3, to evaluate their accuracy for simulating observed soil moisture data. The BC, CA and vG functions and associated parameters (Rawls *et al*. 1992) are listed in Table 3. The soil hydraulic parameters (Rawls *et al*. 1982) of RA are listed in Table 4. The PTFs (Cosby *et al*. 1984) of CO are given as follows:

$$\begin{aligned}
\varphi &= 48.9 - 0.126 \times \text{sand\%} \\
K_s &= 60.96 \times 10^{(-0.884+0.0153\times\text{sand\%})} \qquad (2) \\
b &= 2.91 + 0.159 \times \text{clay\%}
\end{aligned}$$

where ϕ [%V/V], K_s (cm/d) and b (dimensionless) are the soil porosity, soil saturated hydraulic

Table 2 Soil PSD and soil texture at six SCAN sites.

Site	Simulation period*	Depth (cm)	Sand (%)	Clay (%)	Rock (%)	Soil texture
AL2053	12/1/07–2/29/08	0 – 10	7.0	31.5	6	Silty clay loam
		10 – 23	5.8	26.3	1	Silt loam
		23 – 48	4.3	38.6	1	Silty clay loam
		48 – 69	5.4	36.0	1	Silty clay loam
AL2057	12/1/07–2/29/08	0 – 20	29.2	22.9	35	Loam
		20 – 46	24.3	32.3	14	Clay loam
		46 – 69	20.9	41.3	6	Clay
AL2113	12/1/07–2/29/08	0 – 15	48.8	8.1	5	Loam
		15 – 25	42.1	14.3	5	Loam
		25 – 41	43.9	16.7	4	Loam
		41 – 58	41.6	24.6	2	Loam
AR2030	12/1/05–2/28/06	0 – 13	9.7	12.4	0	Silt loam
		13 – 28	7.6	15.1	0	Silt loam
		28 – 48	7.3	18.7	0	Silt loam
		48 – 69	6.1	18.6	0	Silt loam
AR2090	12/1/07–2/29/08	0 – 20	34.8	4.1	0	Silt loam
		20 – 30	34.9	4.2	0	Silt loam
		30 – 43	36.6	4.2	0	Silt loam
		43 – 76	24.6	4.1	0	Silt loam
GA2027	12/1/06–2/28/07	0 – 64	88.1	2.8	6	Sand

* mm/dd/yy.

Table 3 Soil ψ–θ and K–θ relationships.

	BC	CA	vG
K(θ)	$K_s\left(\frac{\theta-\theta_r}{\phi-\theta_r}\right)^{3+2b}$	$K_s\left(\frac{\theta}{\phi}\right)^{3+2b}$	$K_s\left(\frac{\theta-\theta_r}{\phi-\theta_r}\right)^{\frac{1}{2}}\left\{1-\left[1-\left(\frac{\theta-\theta_r}{\phi-\theta_r}\right)^{\frac{1}{m}}\right]^m\right\}^2$
ψ(θ)	$\psi_b\left(\frac{\theta-\theta_r}{\phi-\theta_r}\right)^{-b}$	$\psi_b\left(\frac{\theta}{\phi}\right)^{-b}$	$\psi_b\left[\left(\frac{\theta-\theta_r}{\phi-\theta_r}\right)^{-1/m}-1\right]^{1/n}$

K_s: soil saturated hydraulic conductivity [L/T]; b: pore-size distribution index [-]; θ_r: residual soil moisture content [%V/V]; ϕ: porosity [%V/V]; ψ_b: bubbling pressure head [L]; $m = 1/(1 + b)$; $n = 1 + 1/b$.

Table 4 The RA soil hydraulic property look-up table (Rawls *et al*. 1982).

Soil texture	K_s (cm/h)	ϕ (%)	θ_r (%)	ψ_b (cm)	b
Sand	21.0	43.7	2.0	−7.26	1.44
Loamy sand	6.11	43.7	3.5	−8.69	1.81
Sandy loam	2.59	45.3	4.1	−14.66	2.65
Loam	1.32	46.3	2.7	−11.15	3.97
Silt loam	0.68	50.1	1.5	−20.76	4.27
Sandy clay loam	0.43	39.8	6.8	−28.08	3.13
Clay loam	0.23	46.4	7.5	−25.89	4.13
Silty clay loam	0.15	47.1	4.0	−32.56	5.65
Sandy clay	0.12	43.0	10.9	−29.17	4.48
Silty clay	0.09	47.9	5.6	−34.19	6.67
Clay	0.06	47.5	9.0	−37.30	6.06

conductivity and pore-size distribution index, respectively. Note that residual soil moisture content is one of the parameters that appears in both the BC and vG functions (see Table 3). Because residual soil moisture content was not given in CO's PTFs (i.e. equation (2)), in this paper we apply the residual soil moisture from RA's soil hydraulic property look-up table to CO (i.e. Table 4). Therefore, hereafter we use CO* to represent all cases using residual soil moisture (as determined from RA's look-up table), while all other parameters are based on CO's PTFs.

To solve equation (1), we also re-arrange equation (1) as follows:

$$\frac{\partial\theta}{\partial t} = -\frac{\partial K(\theta)}{\partial z} + \frac{\partial K(\theta)}{\partial z}\frac{\partial\psi(\theta)}{\partial z} + K(\theta)\frac{\partial^2\psi(\theta)}{\partial z^2} \tag{3}$$

and then discretize equation (3) in the vertical direction:

$$\begin{aligned}\frac{\partial\theta_i}{\partial t} = {}& \frac{K(\theta_{i+1}) - K(\theta_{i-1})}{2\Delta z} \\ &+ \frac{[K(\theta_{i+1}) - K(\theta_{i-1})][\psi(\theta_{i+1}) - \psi(\theta_{i-1})]}{(2\Delta z)^2} \\ &+ K(\theta_i)\frac{[\psi(\theta_{i+1}) - 2\psi(\theta_i) + \psi(\theta_{i-1})]}{(\Delta z)^2}\end{aligned} \tag{4}$$

where Δz is the vertical interval and i is the index of the soil layer. In this study, we solve soil moisture between 10 and 50 cm using equation (4). The observed soil moisture values at 10 and 50 cm are used as the upper and lower boundary conditions, and the vertical interval Δz is 1 cm. The time step is 1 hour, and the simulation period is from 1 December to 28 (or 29) February. The observed soil moisture values at 20 cm are used to assess which method most accurately simulates soil moisture by computing the root mean square error (RMSE) and correlation coefficient (r^2) between the simulated and observed soil moisture at 20 cm, given as follows:

$$\begin{aligned}\text{RMSE} &= \sqrt{\frac{\sum_{i=1}^{n}(\widehat{\theta}_i - \theta_i)^2}{n}} \\ r^2 &= \frac{\sum_{i=1}^{n}\left[(\widehat{\theta}_i - \bar{\widehat{\theta}})(\theta_i - \bar{\theta})\right]^2}{\sum_{i=1}^{n}(\widehat{\theta}_i - \bar{\widehat{\theta}})^2\sum_{i=1}^{n}(\theta_i - \bar{\theta})^2}\end{aligned} \tag{5}$$

where n is the number of data points, and $\widehat{\theta}_i$, θ_i, $\bar{\widehat{\theta}}$, and $\bar{\theta}$ are simulated, observed, mean simulated and mean observed soil moisture, respectively. We used linear regression methods (GraphPad Software, Inc., http://www.graphpad.com) to test whether the slopes and intercepts associated with the correlation coefficients computed for simulated *vs* observed soil moisture differed significantly ($P < 0.05$) among the six hydraulic functions and associated parameters, i.e. BC-RA, CA-RA, vG-RA, BC-CO, CA-CO and vG-CO.

4 SIMULATION RESULTS AND DISCUSSION

The time series plots of the simulated and observed soil moisture at 20 cm at six SCAN sites using six different combinations of soil hydraulic functions and soil parameters are shown in Fig. 1. The RMSE and r^2 between the simulated and observed soil moistures at 20 cm for each case are listed in Tables 5 and 6, respectively. According to the plots of the average RMSE and r^2 shown in Fig. 2, we found that, in most cases, the PTFs of RA simulated soil moisture more accurately than those of CO ($P < 0.01$ in 11 of 18 cases across all six sites). Although the average RMSE of the simulated soil moisture using the vG functions is slightly less than those using either the BC or the CA functions, the average r^2 associated with the vG function is only ~0.5, as compared to ~0.75 for the BC and CA functions. In the following sub-sections we describe a series of site-by-site comparisons, which we conducted to test and better understand the effects of the combination of soil hydraulic functions and soil parameters on soil moisture simulation.

4.1 RA soil parameters *vs* CO pedotransfer functions

At each site, there are three pairs of simulated results, i.e. BC-RA *vs* BC-CO*, CA-RA *vs* CA-CO and vG-RA *vs* vG-CO*. Figure 3 shows the RMSE and r^2 of each case. Based on the RMSE values in Fig. 3, we found that, among 18 cases across six sites, there are 11 cases (61%) for which RA simulates observed soil moisture more accurately than CO (mean improvement in RMSE = 23%; range = 94% to –47%). However, except at the AL2035 site, the difference in RMSE between RA and CO or CO* is less than 2%V/V. One interesting point is that in 12 cases (67%), CO's PTFs are associated with a significantly higher correlation coefficient ($P < 0.01$). However, at GA2027, a sandy soil site, RA's soil parameters produced a much higher correlation coefficient than CO's PTFs ($P < 0.01$).

4.2 Influences of residual soil moisture

With regard to the BC and CA functions (see Table 3), it is important to note that these two relationships are fundamentally the same, except that BC includes residual soil moisture and CA sets residual soil moisture equal to zero. Furthermore, for each site, there are two pairs of simulated results that are related to this issue (i.e. BC-RA *vs* CA-RA and BC-CO* *vs* CA-CO), and, consequently, there are 12 cases for us to study the influence of residual soil moisture in the soil hydraulic functions. The RMSEs and the correlation coefficients of these 12 cases are shown in Fig. 4. Regardless of whether we used the RA soil parameters or the CO PTFs, the difference in RMSE between BC and CA is always less than 1%V/V. Thus, although the regression lines for predicted *vs* observed soil moisture for these two PTFs are generally significantly different ($P < 0.05$), there is a negligible absolute difference in the simulated soil moisture whether using soil ψ–θ and K–θ relationships with the residual soil moisture (i.e. BC), or without the residual soil moisture (i.e. CA). This was true even at AL2057, where soil texture is clay loam from 20 to 46 cm and the residual soil moisture of clay loam is 7.5 %V/V (much greater than zero) according to the RA soil hydraulic parameters (see Table 3). According to Fig. 4, BC is only slightly better than CA in terms of the RMSE (<1%V/V), while BC is slightly worse than CA in terms of the correlation coefficient ($P < 0.01$).

4.3 Comparison between the BC and vG functions

In Section 4.1, we showed that the RA PTFs could more accurately ($P < 0.01$) predict soil moisture than the CO PTFs. In Section 4.2, we also found that the effect of including residual soil moisture in the soil hydraulic functions on soil moisture simulation is negligible, i.e. although statistically significant ($P < 0.05$), the absolute difference in simulated soil moisture between the BC and CA functions is small (<1%V/V). Therefore, for this part of the study, we carried out a comparison between only BC-RA and vG-RA. Because there is only one pair of BC-RA *vs* vG-RA at each site, we have six cases to study the difference between the BC and vG functions. Figure 5 shows the RMSE and r^2 values of these six cases. Among these six sites, only at two sites (AL2053 and AL2057) is the RMSE of simulated soil moisture for vG-RA less than that for BC-RA. Comparing

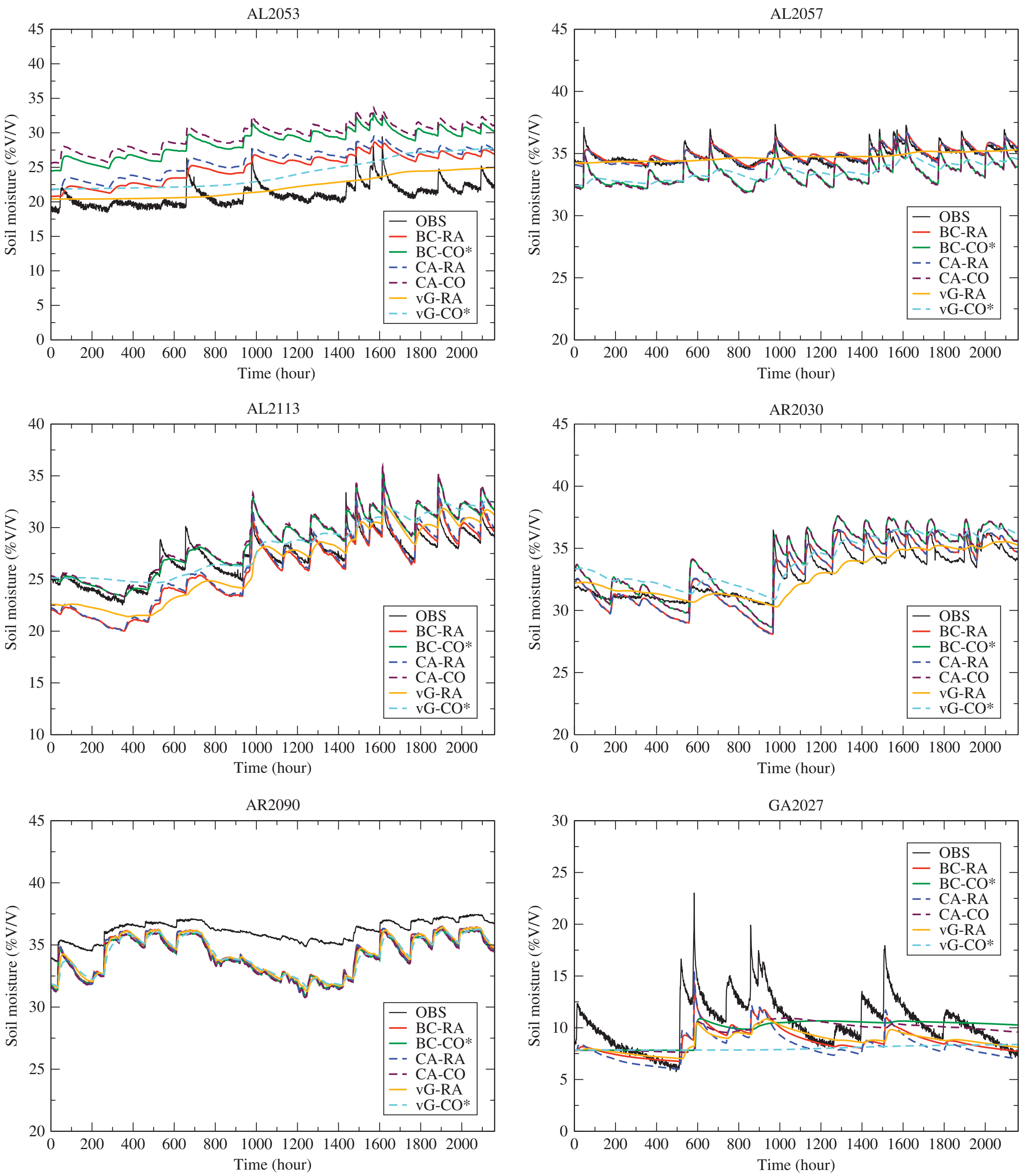

Fig. 1 Time series plots of the observed and simulated soil moisture.

the correlation coefficients, we find that BC-RA is always better than vG-RA ($P < 0.0001$ in all six cases). Furthermore, re-checking the time series plots of the simulated and observed soil moisture in Fig. 1, we find that vG always filters, or smoothes, the high-frequency variation in the observed soil moisture more strongly than BC. Taken together, these results show that BC more accurately predicts observed soil moisture dynamics than vG.

We hypothesize that this filtering effect is due to the comparatively small hydraulic conductivity value at any given soil moisture content given by vG's K–θ

Table 5 The RMSE of the simulated soil moisture.

Site	BC-RA	CA-RA	vG-RA	BC-CO*	CA-CO	vG-CO*
AL2053	4.09	4.90	1.79	7.64	8.55	3.47
AL2057	2.84	2.89	1.90	1.50	1.57	1.80
AL2113	2.01	1.87	3.60	1.84	1.93	1.90
AR2030	0.98	0.99	1.13	1.37	1.38	1.43
AR2090	1.38	1.41	1.50	2.27	2.29	2.09
GA2027	2.35	2.55	2.65	2.48	2.48	3.48
Average	2.28	2.44	2.10	2.85	3.03	2.36

CO* represent all cases as residual soil moisture, as determined from the RA look-up table, while all other parameters are based on the CO PTFs.

Table 6 The correlation coefficient (r^2) of the simulated soil moisture.

Site	BC-RA	CA-RA	vG-RA	BC-CO*	CA-CO	vG-CO*
AL2053	0.58	0.61	0.36	0.68	0.71	0.36
AL2057	0.85	0.85	0.43	0.89	0.89	0.35
AL2113	0.79	0.90	0.51	0.89	0.90	0.62
AR2030	0.88	0.88	0.66	0.90	0.90	0.74
AR2090	0.85	0.85	0.72	0.84	0.84	0.85
GA2027	0.70	0.84	0.39	0.10	0.13	0.01
Average	0.78	0.82	0.51	0.72	0.73	0.49

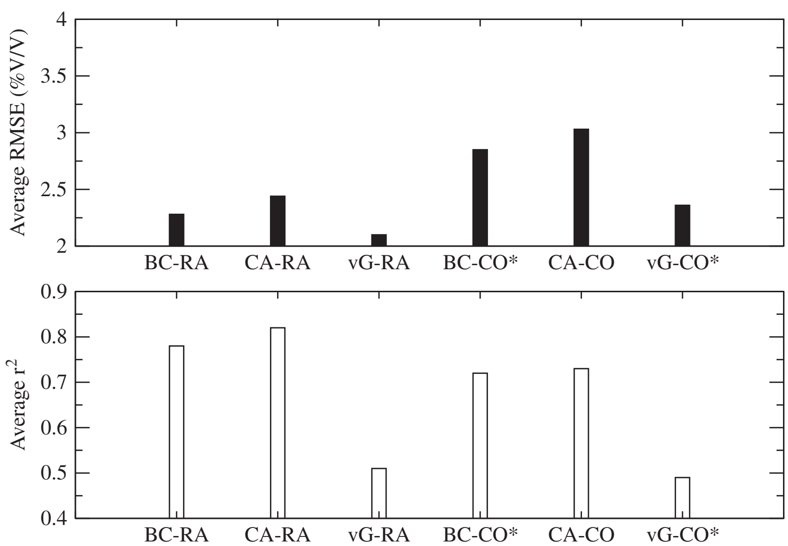

Fig. 2 Average RMSE and correlation coefficient between the simulated and observed soil moisture at 20 cm at six SCAN sites using six different combinations of soil hydraulic functions and soil parameters.

relationship (Fig. 6). For a given soil moisture content, the vG function always gives the smallest K value among the BC, CA and vG functions (Fig. 6). To further test this, we carried out a Fast Fourier Transform (FFT) of the simulated and observed soil moisture. The resulting power spectrum at each site is shown in Fig. 7. The power spectrum is a plot of the power of the signal (i.e. simulated or observed soil moisture in this study) falling within given frequency bins, such that a high spectrum power in a frequency bin indicates a strong variation in the signal in that frequency bin, and low spectrum power indicates low (smoother) signal variation. Figure 7 shows that, across all frequency bins and sites, the spectral power of observed soil moisture is almost always greater than that for simulated soil moisture. Averaged across all six sites, the spectral power of simulated soil moisture for the vG-RA and BC-RA methods is 36 and 17% lower, respectively, than observed values. Furthermore, the spectral power of BC-RA is

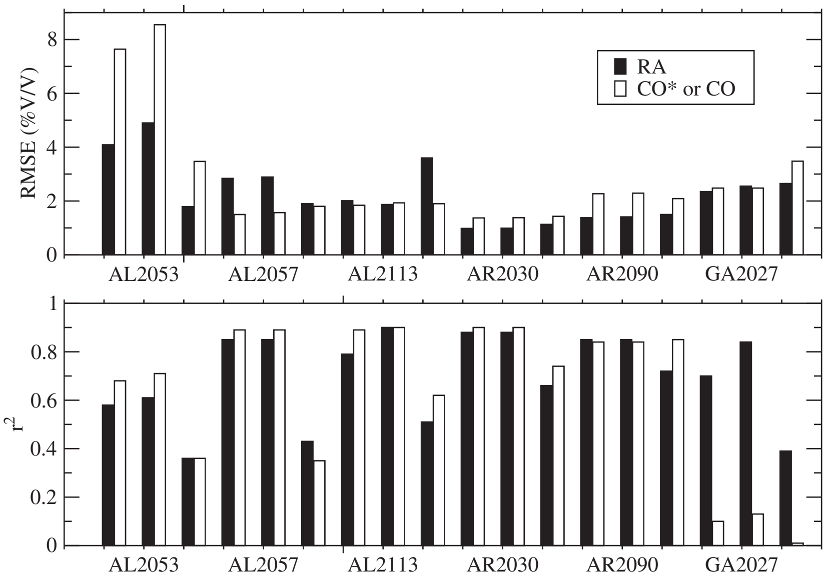

Fig. 3 Comparison of RMSE and correlation coefficient, r^2, of the simulated soil moisture between using the RA soil hydraulic parameters and the CO PTFs.

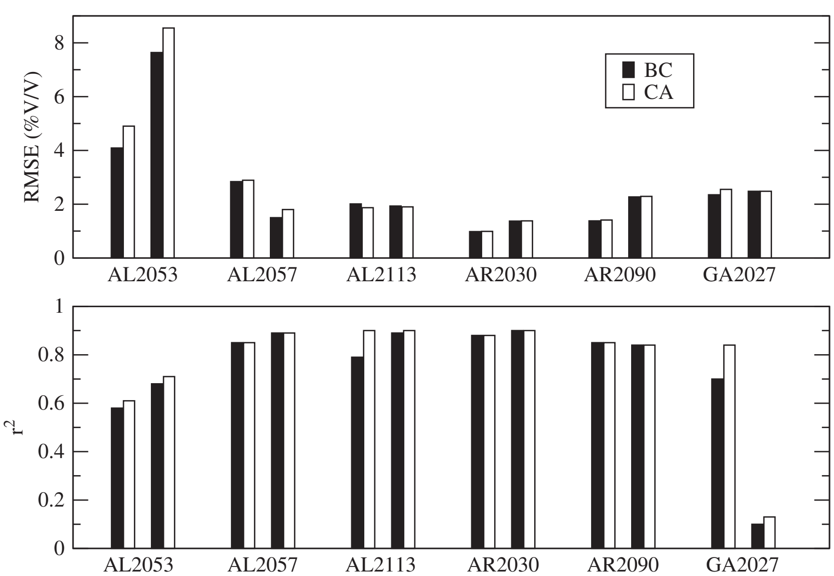

Fig. 4 Comparison of RMSE and correlation coefficient, r^2, of the simulated soil moisture between using the BC and CA functions.

significantly greater ($P < 0.02$ or less across sites) than that of vG-RA. In other words, vG-RA filters the high-frequency signals (i.e. frequency > 1 month^{-1}) in the soil moisture more strongly than does BC-RA. This excessive filtering characteristic of vG-RA is also reflected in the lower correlation coefficients compared to BC-RA ($P < 0.0001$; Fig. 5). Thus, the FFT test reveals why, at any given soil moisture content, the vG always gives the smallest hydraulic conductivity (i.e. the smallest vertical drainage) and thus suppresses vertical communication between upper and lower soil layers.

Although a filtering effect on the simulated soil moisture is also apparent for the BC function, it is much less pronounced than for the vG function (Figs 1 and 7). This raises the question of whether there may be additional, more fundamental explanations for why the high-frequency signals in the simulated soil moisture are filtered, regardless of whether the BC or vG functions are used. For example, is

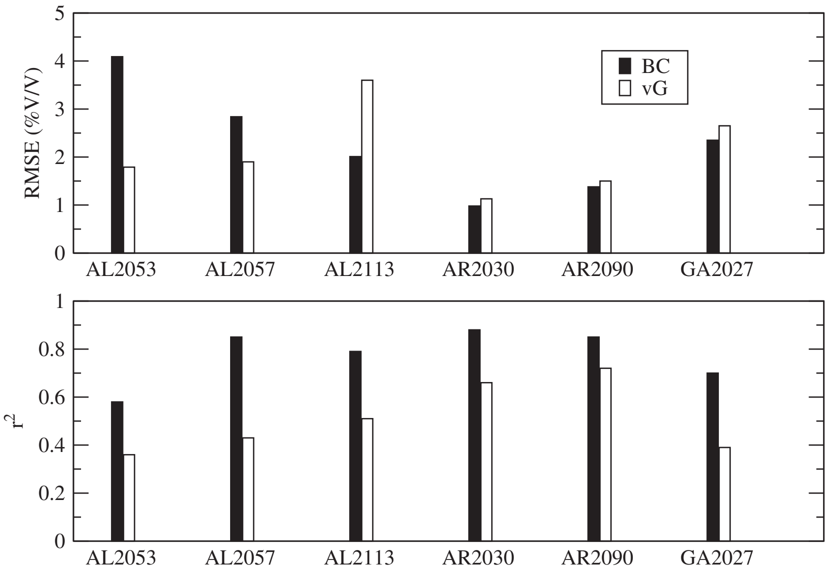

Fig. 5 Comparison of RMSE and correlation coefficient, r^2, of the simulated soil moisture between using the BC and vG functions.

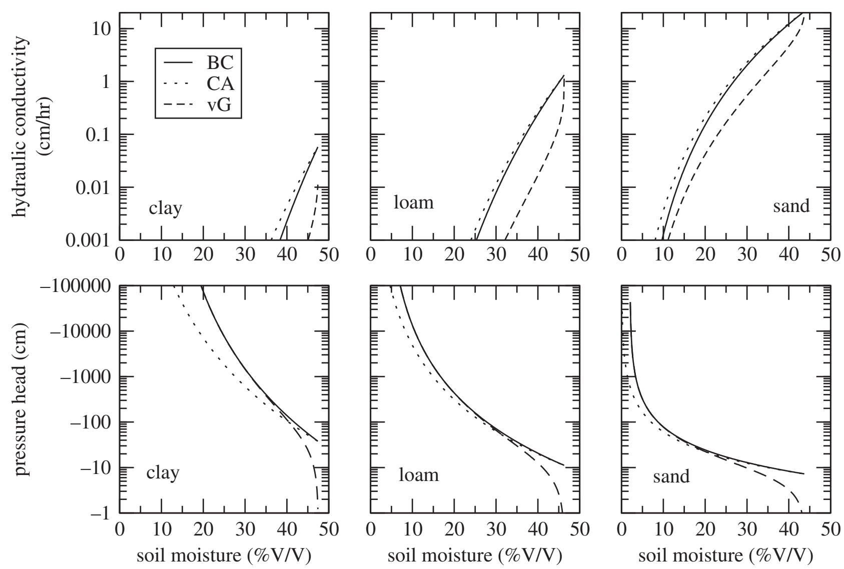

Fig. 6 (a) Comparison of BC, CA and vG K–θ ; and (b) the ψ–θ relationships for sand, loam and clay.

this due to the omission of soil coarse fragments (i.e. rock content) or macropores in the moisture functions? To investigate this issue, we carried out two sets of simulations. One set included rock content in the soil hydraulic conductivity and retention relationships. The second set of simulations considered effects of soil macropores.

4.4 Effect of rock content

Coarse fragments (>2 mm in size) in the soil could reduce soil porosity and soil saturated hydraulic conductivity (Rawls *et al*. 1992). According to Rawls *et al*. (1992), the porosity and soil saturated hydraulic conductivity should be multiplied by the rock content adjustment (RCA) term, given as follows:

$$\text{RCA} = 1 - \text{rock\%} \ \times 0.01 \tag{6}$$

In our study sites, only four sites (AL2053, AL2057, AL2113 and GA2027) have rock contents greater than 0%. We applied the correction term to these four sites and carried out simulations with the adjusted soil saturated hydraulic conductivity and porosity. However, among these four sites, the rock content

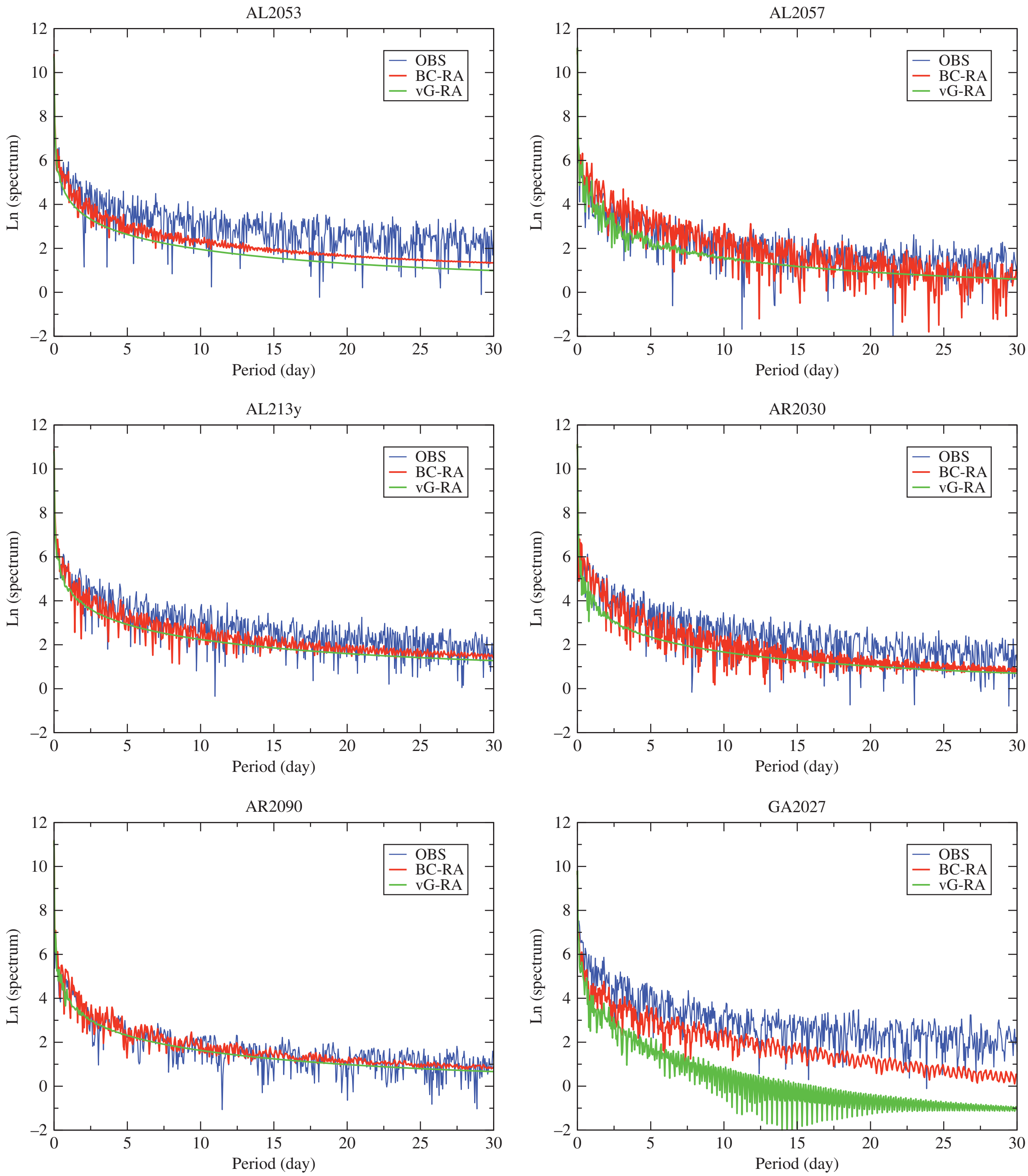

Fig. 7 Spectrum plots of the observed and simulated soil moisture at 20 cm at six SCAN sites.

adjustment (RCA) cannot be applied to AL2057, because the adjusted soil porosity at AL2057 in the layer between 0 and 20 cm is 30.1 (%V/V) and the observed soil moisture at 10 cm in some hours are larger than this adjusted soil porosity. The results for sites AL2053, AL2113, and GA2027 are listed in Table 7. Although the RMSE values for half of the six cases decreased and those for the other half increased, in all cases the absolute changes were negligible (±0.5%V/V). Thus, the results indicate that the effect of rock content on soil moisture simulation can be ignored.

Table 7 Difference in the RMSE and r^2 of simulated soil moisture between BC-RA with rock content adjustment (RCA) and without RCA, and between vG-RA with RCA and without RCA.

Site	BC-RA with RCA – BC-RA without RCA		vG-RA with RCA – vG-RA without RCA	
	RMSE	r^2	RMSE	r^2
AL2053	0.02	0.07	2.15	0.03
AL2113	−0.11	0.11	−0.41	0.25
GA2027	0.03	0.07	−0.04	0.10

4.5 Effect of macropores

Macropores are large-diameter conduits in the soil, created by plant roots, soil cracks, soil fauna, or bacterial activity. Macropores increase the soil hydraulic conductivity and contribute to rapid movement of water and solutes through the soil. To include the effects of macropores in soil water drainage, a dual-porosity and dual-permeability model is often used (e.g. Gerke and van Genuchten 1996). In addition to the fraction of macropores, some geometric characteristics of the macropores are needed for the dual-porosity and dual-permeability model. However, it is difficult to measure the macropores' geometric characteristics. One alternative and much simpler method is to multiply the saturated soil hydraulic conductivity by a factor between 1 and 100 (e.g. Braun and Schädler 2005). This macropore correction factor (MCF) is often calibrated through a sensitivity study.

In this study, we applied three macropore correction factors (5, 10 and 100) to each site, i.e. we solved the Richards equation using the BC-RA method with three adjusted soil saturated hydraulic conductivities: $5K_s$, $10K_s$, and $100K_s$, where K_s is soil saturated hydraulic conductivity determined based on the RA soil hydraulic parameters (Rawls *et al*., 1982). Figure 8 shows the RMSE and r^2 values of the simulated soil moisture when using the macropore-adjusted K_s *vs* the original K_s. As shown in Fig. 8, the improvement in the RMSE of the simulated soil moisture for all six sites is insignificant ($<0.5\%$V/V) when a macropore correction factor (MCF) is applied to the soil saturated hydraulic conductivity. However, the r^2 improved by >0.1 at AL2053, AL2113 and GA2027. One possible reason for these improved correlation coefficients is that multiplying soil K_s by the MCF enhances the communication (i.e. drainage and diffusion) between top and bottom soil layers, and thus accounts for vertical changes in soil moisture.

Why did the MCF adjustment to K_s not improve the accuracy of the simulated soil moisture? It is well established that soil macropores can substantially increase soil hydraulic conductivity, and not just the saturated hydraulic conductivity, K_s. Obviously, an increase in K_s (through a MCF multiplier) will increase soil hydraulic conductivity K according to the BC hydraulic function, as follows:

$$K = K_s S^{3+2b} = K_s \left(\frac{\theta - \theta_r}{\phi - \theta_r}\right)^{3+2b} \tag{7}$$

where S is soil saturation and b is the soil pore-size distribution index, as soil moisture is less than the saturated soil moisture content. Thus, a large value of b in the scaling exponent, $3 + 2b$, in equation (7) will cause a pronounced exponential decay of soil hydraulic conductivity. According to the RA soil parameters (see Table 4), the b values of 11 soil texture classes are between 1.44 and 6.67 and thus $3 + 2b$ in equation (7) is in the range of 5.88 to 16.34. If soil saturation is 0.5, the soil hydraulic conductivity K is between 1.2×10^{-5} K_s and $0.02K_s$. If we apply a MCF $= 2$ to adjust K_s, then K is between 2.4×10^{-5} K_s and $0.04K_s$. If we halve the b value, then K is between 1.2×10^{-3} K_s and $0.05K_s$. The above simple calculation demonstrates that, in a power function like equation (7), the more sensitive parameter is the scaling exponent (i.e. $3 + 2b$). Therefore, we could argue that the pore-size distribution index, b, in the soil hydraulic conductivity functions is the most sensitive parameter among soil hydraulic parameters, i.e. K_s, b, ϕ and θ_r. In fact, Ek and Cuenca (1994) found that b is the most sensitive hydraulic parameter.

To test the sensitivity of the simulated soil moisture to b, we carried out two sensitivity tests at each site: $0.5b$, and $2b$. Based on the plots of the RMSE and r^2 values shown in Fig. 9, we find that r^2 decreases (increases) when we double (halve) the b value at AL2053, AL2113 and GA2027; at three other sites, r^2 is not sensitive to b. However, the effect of the b value on the RMSE is not monotonic. At sites AL2053 and

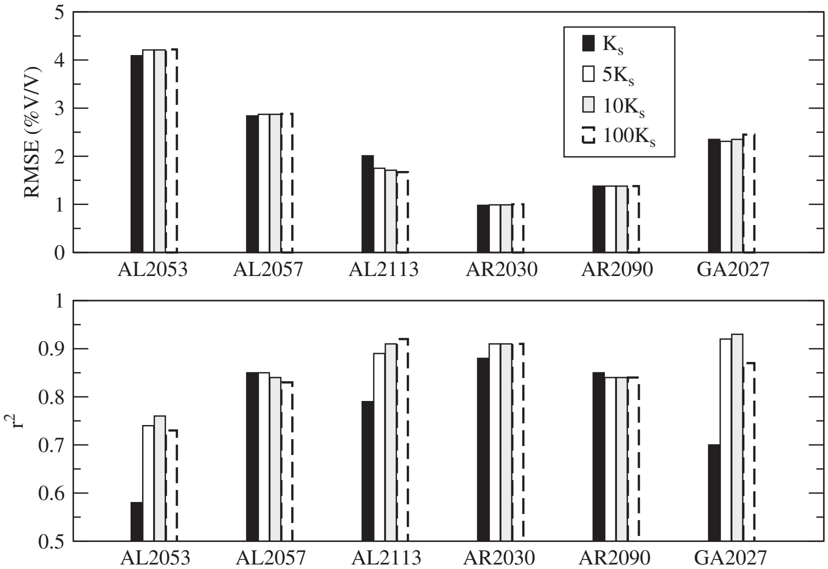

Fig. 8 Sensitivity test of the simulated soil moisture to soil saturated hydraulic conductivity, K_s.

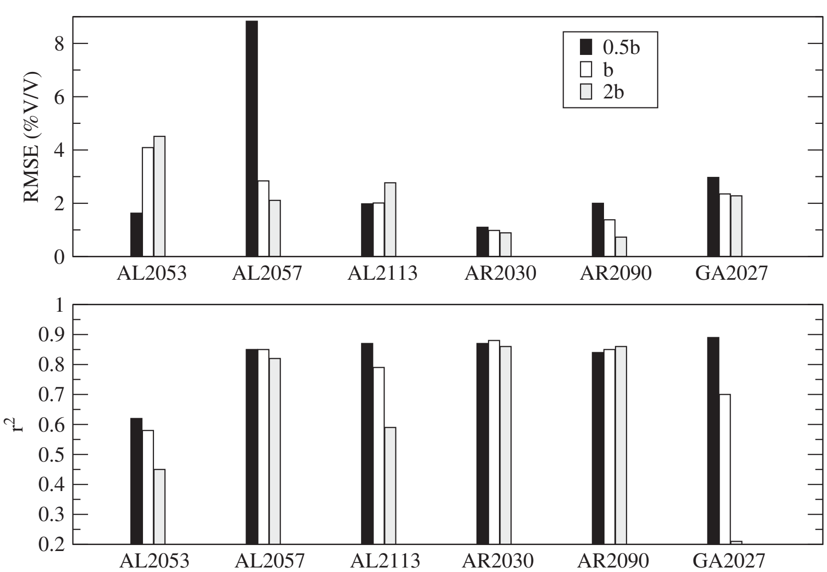

Fig. 9 Sensitivity test of the simulated soil moisture to the soil pore size distribution index *b*.

AL2113, the RMSE values were reduced by halving the *b* value, and at four other sites (AL2057, AR2030, AR2090 and GA2027), the RMSE values were reduced by multiplying *b* by 2. The improvement in RMSE is as high as 2.46 at site AL2053. These results indicate that the simulated soil moisture is more sensitive to *b* than to K_s, and that applying only a macropore factor to K_s is insufficient.

5 SUMMARY

In this paper, we examined the effects of different soil hydraulic functions and parameters on the accuracy of soil moisture simulations. Unlike other studies, this study took a unique approach to eliminate the effects of evaporation and transpiration so that we could isolate and focus on just the effects of soil hydraulic functions and soil parameters on modelling soil moisture dynamics. By comparing simulated and observed soil moisture dynamics at six field sites, we have drawn the following conclusions:

(1) The simulated soil moisture using the RA soil parameters (Rawls *et al*. 1982) are more accurate than using the CO PTFs (Cosby *et al*. 1984). Although the Rawls *et al*. look-up table is slightly better, the errors in the simulated soil

moisture at some sites are comparable to the measurement error, e.g. at AL2053. The uncertainty in the hydraulic properties of Rawls *et al*. is one reason; another is that, even for the same soil texture, there is a wide range of variation in soil PSD (i.e. sand and clay contents). To reduce such uncertainty, some efforts are needed to develop accurate pedotransfer functions for each soil texture, rather than a set of universal PTFs like Cosby *et al*. (1984).

(2) Residual soil moisture in the soil hydraulic functions plays a negligible role in affecting soil moisture simulations. This indicates that we can set the residual soil moisture content to zero in the soil hydraulic functions without creating a large error in the simulated soil moisture.

(3) Although the overall errors in the simulated soil moisture using the vG functions are slightly less than those using the BC or CA functions, the vG functions excessively filter high-frequency variations because, at any given soil moisture content, the vG functions always give the smallest hydraulic conductivity, and thus unrealistically reduce the movement of water between the upper and lower soil layers. The BC and CA functions more accurately represent this interlayer communication. Therefore, we recommend BC-RA or CA-RA for modelling soil moisture.

(4) Adjusting soil hydraulic conductivity and soil porosity by a rock content correction term could not improve the accuracy of the simulated soil moisture, and at some sites the accuracy became even worse.

(5) Both the RA soil parameters and the CO PTFs were obtained through laboratory testing of soil samples collected in the field. However, during the process of collecting and transporting soil samples, the macropores in soil samples could be damaged to some degree. Therefore, the RA soil moisture and CO's PTFs likely do not represent actual field soil hydraulic properties and underestimate soil hydraulic conductivity. We evaluated the effects of a commonly-used approach for adjusting soil saturated hydraulic conductivity (K_s) by a macropore correction factor (MCF). Through a series of sensitivity tests, we found that only adjusting K_s by the MCF is insufficient, because soil hydraulic conductivity is more sensitive to the soil pore size distribution index b (which is the scaling exponent of the power function of soil hydraulic conductivity) than it is to K_s. In summary, our results show that the assumptions underlying commonly-used soil hydraulic functions and parameters have significant effects on the accuracy of soil moisture predictions, and that the most accurate options are the BC-RA and CA-RA methods with an added variation that also addresses the effects of macropores, in particular, the soil pore size distribution.

The focus of this paper was to introduce a new and effective approach for identifying optimal soil hydraulic functions and parameters through comparing observed and simulated soil moisture. Based on the results of this study, we argue that more effort is needed to measure soil hydraulic parameters and obtain soil hydraulic functions directly in the field, rather than in the laboratory, because during the process of collecting and transporting soil samples, macrospores in soils could be damaged to some degree. This study also provides a basis for obtaining a complete set of optimal hydraulic parameters for 11 soil texture classes, which is the subject of a future study.

Acknowledgements This research was partially supported by the University of North Texas (UNT) Research Initiative Grant (RIG) (Pan). The information in this document has been funded in part by the US Environmental Protection Agency. It has been subjected to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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