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Optimizing Soil Hydraulic Parameters in RZWQM2 under Fallow Conditions

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Robust estimation of soil hydraulic parameters is essential for predicting soil water dynamics and related biogeochemical processes; however, uncertainties in estimated parameter values limit a model's ability for prediction and application. In this study, methods of global analysis (Latin hypercube sampling, LHS) and gradient-based optimization (PEST, parameter estimation software) were explored to calibrate soil hydraulic parameters in the Root Zone Water Quality Model (RZWQM2). Six methods of estimating Brooks–Corey parameters of the soil water retention curve and saturated hydraulic conductivity were evaluated to simulate daily soil water dynamics under fallow conditions in eastern Colorado. The calibrated soil hydraulic parameters showed similar trends with soil depth for the different estimation methods in RZWQM2 but resulted in large differences between simulated and observed soil water contents. The PEST optimization based on soil type values as initial estimates gave reasonable soil water responses but with some unrealistic soil hydraulic parameters and soil evaporation. Overall, errors in simulated soil water contents were reduced by using LHS to initialize and constrain the PEST parameter space, which also stabilized the cross-validation results. Calibration results using water content measurements at four depths (30, 60, 90, and 150 cm) were similar to results using 10 depths (30, 40, 50, 60, 70, 80, 90, 120, 150, and 170 cm). Calibrating soil hydraulic parameters remains challenging, but the combined calibration procedures (LHS + PEST) with cross-validation can reduce parameter uncertainties and improve model performance.

Abbreviations: BC, Brooks–Corey; GML, Gauss–Marquard–Levenberg; LHS, Latin hypercube sampling; NSME, Nash–Sutcliffe model efficiency; RZWQM2, Root Zone Water Quality Model; SWRC, soil water retention curve.

An agricultural system model is a promising tool to quantify and improve our understanding of soil hydrologic processes and to evaluate and extrapolate various agricultural management practices under different climate and soil conditions (Ahuja et al., 2006; Ma et al., 2007). Model calibration and evaluation are essential for successful model applications. Soil hydraulic properties, including soil water retention and hydraulic conductivity, are the most important parameters in these models that influence the soil water flow and mass balance (Ahuja and Ma, 2002; Ahuja et al., 2006). Laboratory and in situ measurements of these hydraulic parameters are often insufficient, however, for the model input requirements (Mertens et al., 2005; Oliver and Smettem, 2005). Therefore, many pedotransfer functions (Bouma and van Lanen, 1987; Bouma, 1989) have been developed to estimate soil hydraulic parameters by relating the missing parameters to the available basic soil data (Børgesen et al., 2008; Chirico et al., 2007; Twarakavi et al., 2008). Several reviews on the development, application, and evaluation of pedotransfer functions can be found in the literature (Ahuja et al., 1999; Rawls et al., 1991; van Genuchten and Leij, 1992; Wösten et al., 2001). Based on a similar-media concept (Simmons et al., 1979; Warrick et al., 1977), advances in the development of pedotransfer functions and inverse modeling have used surrogate soil data, such as bulk density and soil water content at 33 kPa suction, to estimate the complete

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soil water retention curve (SWRC) of a related soil textural class (Ahuja et al., 1985; Williams and Ahuja, 1992).

The RZWQM2 model (Ahuja et al., 2000) has been applied to many research problems using manual calibration based on experience and expertise. No systematic and repeatable approach for parameter estimation has been applied to RZWQM2 until very recently, when Nolan et al. (2010) used PEST to calibrate RZWQM2. Due to parameter cross-correlations, it is possible that soil and plant parameters have been tuned with compensating effects. Thus, there remains a need to apply a systematic automated approach of parameter estimation to fallow periods with no soil–crop interaction. Soil hydraulic properties estimated during fallow periods should be applicable to the cropped phase, allowing independent estimation of crop parameters later.

Most studies on calibrating the parameters in RZWQM2 did not consider the differences between the parameter estimation methods provided in the RZWQM2 interface (Fang et al., 2008, 2010; Hu et al., 2006; Yu et al., 2006). A recent study showed that these methods for estimating soil hydraulic properties strongly influenced the soil water balance and crop growth results (Ma et al., 2009).

Soil parameters vary in space and time as influenced by soil and climate conditions and management practices (Ahuja et al., 1998; Green et al., 2003; Strudley et al., 2008), which has made it difficult to calibrate these parameters in agricultural system models when few measured field data were available (Ahuja et al., 1999, 2006; Hupet et al., 2004). Nonlinear correlations between these parameters also contribute to the uncertainties (Ahuja et al., 1998; Ahuja and Ma, 2002). Traditional trial-and-error calibration methods are time consuming and subjective and it is difficult to get the best parameter values due to the complex interactions between these parameters in the model.

To cope with these difficulties, many strategies for tackling the above problems, such as decomposition, screening, and space reduction (Shan and Wang, 2009) and some associated automatic calibration procedures have also been developed for parameter estimations (Duan et al., 1992; Madsen et al., 2002; Vrugt et al., 2008). In general, automatic calibration algorithms or procedures can be classified as local or global search strategies (Sorooshian and Gupta, 1995). For example, the gradient-based Gauss–Marquard–Levenberg (GML) procedure, as a local search strategy, was implemented in the PEST software (Doherty, 2004), which has been used widely to calibrate soil hydraulic parameters (Iskra and Droste, 2007; Jhorar et al., 2004; Maneta et al., 2008; Skahill et al., 2009). Such gradient-based methods have been applied in vadose zone hydrology modeling studies (Meadows et al., 2005; Si and Kachanoski, 2000; Romano and Santini, 1999). The typical global search procedures, such as Shuffled Complex Evolution (Duan et al., 1992), genetic algorithms (Wang, 1991), and simulated annealing (Sumner et al., 1997), are also widely applied in hydraulic models (Madsen et al., 2002; Vrugt et al., 2003b). These optimization methods have been applied to optimize soil hydraulic parameters for vadose zone hydrology modeling (Abbaspour et al., 2004; Hupet et al., 2003; Mertens et al., 2005; Vrugt et al., 2003a). Latin hypercube sampling (McKay et al., 1979) continues to be used widely for parameter sensitivity analysis (Christiaens and Feyen, 2002; van Griensven et al., 2006). These different model calibration procedures have been highly efficient in multiple parameter calibrations of hydraulic models with some constraints for application (Beven and Binley, 1992; Duan et al., 1992). More recently developed advanced Markov chain Monte Carlo methods and the global multimethod search algorithm AMALGAM have been explored for estimating the Pareto solution set and posterior probability density function of the parameters (Vrugt et al., 2003b; Vrugt and Robinson, 2007; Wöhling et al., 2008). These methods continue to advance (Vrugt et al., 2009; Huisman et al., 2010) but their application to RZWQM2 is beyond the scope of this study.

In this study, LHS and the GML-based PEST software were used as well-established procedures to calibrate soil hydraulic parameters in RZWQM2 and test different internal parameter estimation methods in combination with these external optimization strategies. High temporal resolution soil water measurements at multiple depths from dielectric probes during fallow periods in a dryland winter wheat (*Triticum aestivum* L.) field in Colorado were used for calibration and evaluation. Six methods for estimating soil water retention and hydraulic conductivity based on the Brooks–Corey (BC) model (Brooks and Corey, 1964) in RZWQM2 were compared.

The specific objectives of the study were to: (i) evaluate and compare six different parameter estimation methods within the RZWQM2 for calibrating soil hydraulic parameters and simulating soil water dynamics across seasons; (ii) test whether the calibration of soil hydraulic properties in RZWQM2 can be improved using different combinations of external procedures (LHS and PEST) for parameter estimation; and (iii) relate parameter variability associated with measured data sets and parameter estimation to soil processes and profile water balance.

MATERIALS AND METHODS

Soil Hydraulic Parameter Estimation Methods within RZWQM2

The RZWQM2 model uses soil horizons to define soil properties, and each horizon has its own soil physical and hydraulic properties. The physical properties are bulk density, particle density, porosity, and texture. Hydraulic properties are defined by the soil water content–matric suction relationship and the unsaturated hydraulic conductivity–matric suction relationship, which are both described by the BC model (Brooks and Corey, 1964) with slight modifications. The BC model was originally developed and validated based on limited soil types but has been widely applied to simulate soil water and nutrient movement and dynamics under various climate and soil conditions using RZWQM2 (and its predecessor, RZWQM) (Ahuja et al., 2000; Ma et al., 2007) and other soil hydrology models.

The BC equations and parameter values are defined here for reference. For water retention, the equations used to relate volumetric soil water content (θ) and matric suction head (ψ, where $\psi > 0$ for negative soil water pressures) are

$$\theta=\theta_s \qquad \text{for } \psi<\psi_b \qquad [1]$$

$$\frac{\theta-\theta_r}{\theta_s-\theta_r}=\left(\frac{\psi}{\psi_b}\right)^{-\lambda} \qquad \text{for } \psi\geq\psi_b \qquad [2]$$

where θ_s and θ_r are saturated and residual soil water contents, respectively, ψ_b is the air-entry water suction (negative "bubbling pressure head"), and λ is the absolute value of the slope of the log(θ)–log(ψ) curve or the pore-size distribution index. Similarly, assuming that the log–log slope of the water retention curve is linearly related to the log–log slope of the unsaturated conductivity curve, the hydraulic conductivity, K, vs. suction head is

$$K(\psi)=K_{sat} \qquad \text{for } \psi<\psi_b \qquad [3]$$

$$K(\psi)=K_{sat}\left(\frac{\psi}{\psi_b}\right)^{-(2+3\lambda)} \qquad \text{for } \psi\geq\psi_b \qquad [4]$$

where K_{sat} is the saturated hydraulic conductivity. Therefore, the "full" set of BC parameters for both water retention and conductivity include K_{sat}, θ_s, θ_r, ψ_b, and λ.

In RZWQM2, several methods are available for estimating the SWRC, such as the one-parameter method from soil water content at 33-kPa soil suction (Williams and Ahuja, 1992) and the two-parameter method from soil water contents at both 33- and 1500-kPa soil suctions (Ma et al., 2009). In the model, K_{sat} can be estimated based on effective porosity (Ahuja et al., 1989) or from soil texture class mean values (Rawls et al., 1982). In this study, six internal methods for estimating the BC parameters were used. These methods were comprised of three methods for estimating water retention parameters and two methods for estimating K_{sat}. For the first method, the relationship between θ and ψ can be written as (Ahuja and Williams, 1991)

$$\ln(\psi)=a+b\ln(\theta-\theta_r) \qquad [5]$$

where $b = -1/\lambda$. Williams and Ahuja (1992) found that

$$a=p+qb \qquad [6]$$

where $p = -0.52$ and $q = 0.67$ for all soil texture classes when ψ is in kilopascals. The value of λ is calculated from θ_s and $\theta_{1/3}$ (soil water content at 33 kPa or 1/3 bar), and then ψ_b is obtained from a and λ, where $a = \ln(B)/\lambda$ and $B = (\theta_s - \theta_r)\psi_b^{\lambda}$ (Williams and Ahuja, 2003). Because a soil water retention curve can be estimated using only $\theta_{1/3}$ (assuming θ_s is measured and $\theta_r = 0$ or a known value), it is called the *one-parameter method*. In this study, θ_s and θ_r are added unknowns, but with smaller bounds.

The second method to estimate a soil water retention curve was based on both $\theta_{1/3}$ and θ_{15} (soil water content at 1500 kPa). From Eq. [5], we can derive two equations:

$$\ln(333)=a+b\ln(\theta_{1/3}-\theta_r) \qquad [7]$$

$$\ln(15{,}000)=a+b\ln(\theta_{15}-\theta_r) \qquad [8]$$

From these two equations, λ is

$$\lambda=\frac{\ln\left[(\theta_{1/3}-\theta_r)/(\theta_{15}-\theta_r)\right]}{\ln(15{,}000/333)} \qquad [9]$$

Because both $\theta_{1/3}$ and θ_{15} are needed for estimating the soil water retention curve, it is called the *two-parameter method*.

The third method was based on the parameters λ, ψ_b, θ_s, and θ_r in RZWQM2. This is called the *full Brooks–Corey parameter method* because all of the parameters for the BC model were used for both water retention and hydraulic conductivity as functions of matric suction. Water content at any suction (e.g., $\theta_{1/3}$ and θ_{15}) can be computed from the full BC model for comparison with the other methods.

Another parameter, K_{sat} (cm h^{-1}), needed for RZWQM2 was estimated initially from the soil texture class based on average soil hydraulic properties (Rawls et al., 1982). Alternatively, based on the formula by Ahuja et al. (1989), K_{sat} was estimated using an improved empirical relationship with effective porosity:

$$K_{sat}=509.4(\theta_s-\theta_{1/3})^{3.63} \qquad [10]$$

In this study, six combinations of soil water retention curve estimation and K_{sat} estimation methods were used (Table 1). The SWRC1K$_{in}$ method is the one-parameter method with K_{sat} as an independent input, while SWRC1K$_{es}$ is the one-parameter method with K_{sat} calculated from Eq. [10]. The SWRC2K$_{in}$ method is the two-parameter method with K_{sat} as independent input, and SWRC2K$_{es}$ is the two-parameter method with K_{sat} calculated from Eq. [10]. The SWRCλK$_{in}$ and SWRCλK$_{es}$ methods are the corresponding full BC parameter methods. All of these estimation methods in RZWQM2 were used for parameter calibrations with the following external optimization methods.

Parameter Optimization Methods

Latin hypercube sampling is a global parameter analysis method (McKay et al., 1979) that samples the joint cumulative density function rather than the joint probability density function as in other Monte Carlo based methods. Latin hypercube sampling produces uniform coverage of the parameter space and is more efficient than the original Monte Carlo sampling method. Other global search methods, such as Markov chain Monte Carlo sampling (Vrugt et al., 2003b; Marshall et

Table 1. Parameter estimation methods used for the soil water retention curve (SWRC) and saturated hydraulic conductivity in RZWQM2, and external optimization procedures using Latin hypercube sampling (LHS) and the PEST parameter estimation program.

Method	K_{sat} independent	K_{sat} estimated from Eq. [10]	Calibration parameters†	Optimization procedures
One-parameter method	SWRC1K$_{in}$	SWRC1K$_{es}$	θ_s, $\theta_{1/3}$, K_{sat}	PEST, LHS, LHS + PEST
Two-parameter method	SWRC2K$_{in}$	SWRC2K$_{es}$	θ_s, $\theta_{1/3}$, θ_{15}, K_{sat}	PEST, LHS + PEST
Full Brooks–Corey method	SWRCλK$_{in}$	SWRCλK$_{es}$	θ_s, λ, ψ_b, K_{sat}	PEST, LHS, LHS + PEST

† θ_s, saturated soil water content (m^3 m^{-3}); $\theta_{1/3}$ and θ_{15}, soil water contents at 33 and 1500 kPa (m^3 m^{-3}); K_{sat}, saturated hydraulic conductivity (cm h^{-1}); λ, pore-size distribution index; ψ_b, air-entry water suction or negative bubbling pressure head (cm).

al., 2004), can be more efficient than LHS, but in this study we used the LHS method mainly to search for initial values and ranges of the soil hydraulic parameters in RZWQM2 for PEST optimizations. The soil hydraulic parameters, θ_s, θ_r, $\theta_{1/3}$, λ, ψ_b and K_{sat}, were sampled with 6000 combinations (simulation runs) for the one-parameter method and the full BC method in RZWQM2. The sampled parameters were then used to run RZWQM2 and ranked based on the simulation results. The best parameter sets and parameter ranges sampled by LHS were used for further calibration using PEST.

The PEST program is a model-independent optimization software (Doherty, 2004) that communicates with a model using its own input and output files without any changes to the model. To optimize the soil hydraulic parameters in RZWQM2, the PAR2PAR utility in PEST was used to calculate and transform the BC or K_{sat} parameter values based on the parameter estimation methods in RZWQM2 as described above. Nolan et al. (2010) applied a similar procedure using PEST in conjunction with RZWQM2. During optimization, PEST varies each parameter from the current estimated values based on the GML method and reruns the model. An important restriction in the GML method is sensitivity to local minima (Gupta et al., 2003; Vrugt et al., 2003a). The initial parameter values and the given ranges of the parameters can affect the calibration result (Hopmans et al., 2002; van Dam et al., 1994). Global sampling to constrain the reasonable parameter ranges can potentially eliminate these problems. In this study, we tested whether the calibration of soil hydraulic parameters in RZWQM2 can be improved by combining the LHS and PEST calibration strategies (LHS + PEST).

The objective function used for PEST optimization is similar to the sum of squared errors between measured and simulated data sets:

$$\Phi=\frac{1}{n}\sum_{i=1}^{n}\left\{w_i\left[O\left(t_i\right)-P\left(F,t_i\right)\right]\right\}^2 \qquad [11]$$

where F is a set of fitting parameters, $O(t_i)$ is the observation at the ith time, $P(F,t_i)$ is the model prediction at the ith time, and w_i is the weighting factor for the ith observation. We only have one observation type (soil water content), and the weighting factor (w_i) was set to 1 for all i.

Experimental Site Description

The field site is part of the Drake Farm located in eastern Colorado (40.61′ N, 104.84′ W) as shown in Fig. 1. The average annual potential evaporation is approximately 1200 mm, while the average annual precipitation is approximately 350 mm. The soils include Wagonwheel loam (a coarse-silty, mixed, superactive, mesic Aridic Calciustept), Colby silt loam (a fine-silty, mixed, superactive, calcareous, mesic Aridic Ustorthent), and a Kim fine sandy loam (a fine-loamy, mixed, active, calcareous, mesic Ustic Torriorthent). Representative soil profiles, including the depths of soil horizons and other basic soil information, were based on an Order-2 NRCS soil survey (Michael Peterson, NRCS, personal communication, 2001). The field was managed with a winter wheat–fallow rotation in alternating strips (approximately 120 m wide). Winter wheat was planted in the fall and harvested in summer (usually mid-July) the following year. After wheat harvest, the strips remained fallow until the second autumn (about 13–14 mo) before being replanted. Fallow strips were typically swept monthly with V-blades to control actively growing weeds. More detailed information on the experimental site can be found in Green et al. (2009). Soil moisture was measured hourly with dielectric capacitance sensors (Sentek EnviroSCAN or EnviroSMART, Sentek Sensor Technologies, Stepney, SA, Australia) from 2002 to 2008 including four fallow periods and four crop seasons. Schwank et al. (2006) provided a detailed description and laboratory characterization of the Sentek capacitance sensors, including the measurement zone in the media around the access tube. All Sentek probes were fully buried such that the probe did not interfere with management practices and cropping patterns directly above each

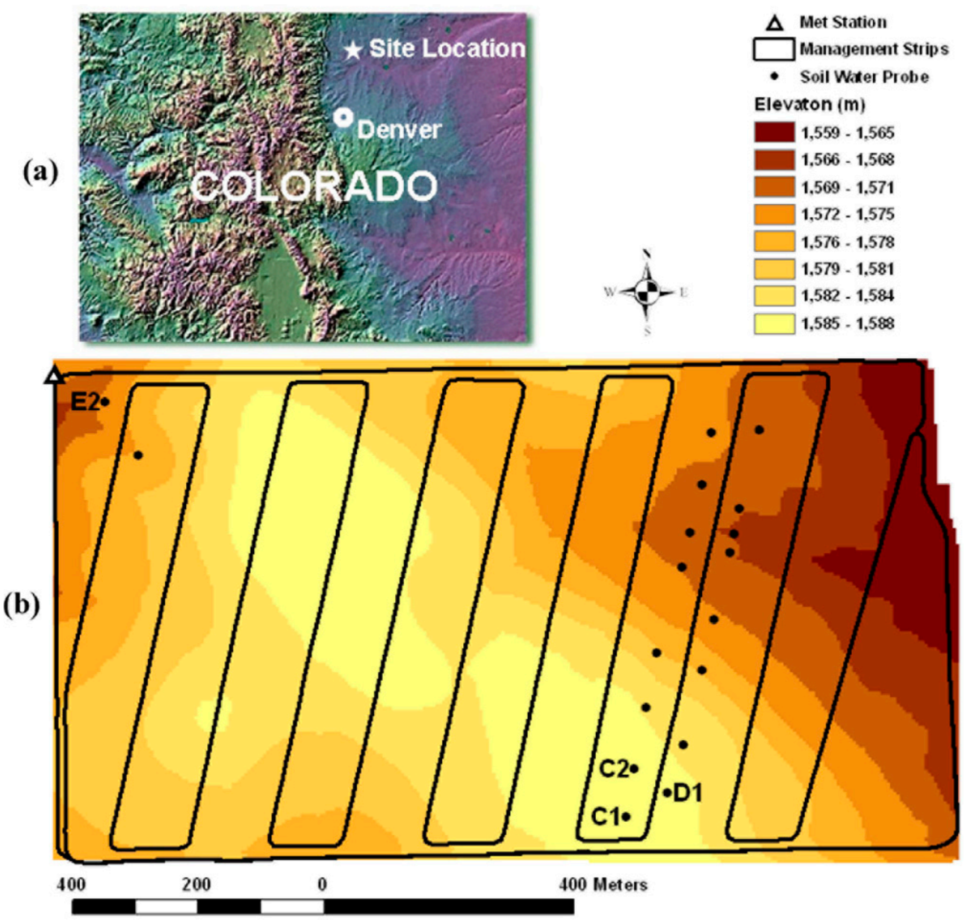

Fig. 1. Site map showing (a) the field site (star) within the state of Colorado, and (b) locations of instruments used to measure profile soil water contents and meteorological data. Only Sites C1, C2, D1, and E2 were simulated in this study. Wheat–fallow rotations were managed in alternating strips (delineated with black lines).

probe. Wires were routed in buried trenches to the dataloggers at the edge of the field.

Each "site" or landscape position fell within one management rotation or the other and was represented by a single in situ EnviroSCAN or EnviroSMART probe with sensors at multiple depths (not replicated within a site). At one site (E2), measurements were centered at 10 depths of 30, 40, 50, 60, 70, 80, 90, 120, 150, and 170 cm (Table 2), where each sensor integrated approximately 10 cm vertically. Three other sites (C1, C2, and D1 in Fig. 1), with measured soil moisture at 30-, 60-, 90-, and 120- or 150-cm depths, were also used for comparing the different calibration procedures. The four sites selected for this study were in landscape positions (summit or crest) where runoff did not accumulate on the surface, and little or no lateral subsurface flow was expected. At the meteorological station in the northwest corner of the field, 12-min climate data including wind, solar radiation, and temperature were measured. These data were averaged to daily values and used as model inputs, along with breakpoint rainfall intensity data (1.5-mm increments).

The measured soil water contents were low during the winter (dry period), increased due to snowmelt and rainfall during the spring and early summer (wet period), and maintained relatively high values during the autumn. Comparing the two fallow periods at Site E2, the soil water contents were lower during the 2002–2003 fallow period than the 2004–2005 fallow period (Fig. 2). Comparing soil water contents at different depths, the soil water at the 30-, 40-, and 50-cm depths showed similar trends (similar mean and standard error values), and similar soil water dynamics were found at the 60-, 70-, and 80-cm depths, at the 90-cm depth, and at the 120-, 150-, and 170-cm depths (Table 2). This result indicated that the vertical soil layers could be separated into four depths (15–55, 55–85, 85–105, and 105–170 cm) plus the surface layer (0–15 cm), which is consistent with the soil survey data and field observations.

Model Calibration and Evaluation

Two fallow periods at Site E2 were alternated for model calibration and evaluation, i.e., cross-validation (Table 2). The same approach was applied to simulate Sites C1, C2, and D1, but the fallow periods differed among them. For the other three sites (Fig. 1), the moisture data sets included Fallow 1 (2006–2007 at C1 and C2 and 2007–2008 at D1) and Fallow 2 (2002–2003 at C1 and C2 and 2005–2006 at D1). At Site E2, we also compared the calibration results with the observations at 10 depths (30, 40, 50, 60, 70, 80, 90, 120, 150, and 170 cm) or at four depths (30, 60, 90, and 120 cm) for the site.

Four stepwise approaches for calibrating soil hydraulic parameters in RZWQM2 were tested: (i) the default parameter values from RZWQM2 based on soil type (from soil surveys) were used based on Rawls et al. (1982); (ii) PEST optimization, where the initial values and ranges of these parameters were estimated by RZWQM2 based on soil types, and all six internal parameter estimation methods were used; (iii) LHS was used to sample the full range of parameters for the one-parameter method and the full BC parameter method; and (iv) based on the LHS analysis, further optimization using PEST for these parameters was performed across the six methods, where initial values and boundaries of these parameters for the two-parameter methods (SWRC2K$_{in}$ and SWRC2K$_{es}$) were based on LHS search results of the full BC method. Across these parameter estimation methods in RZWQM2, the selected initial parameter values and boundaries were slightly different. For all four steps, the different temporal data sets (Fallow 1 and Fallow 2) were compared. After that, we further compared the three different calibration procedures (ii–iv) with the measured soil moisture data from other three sites.

Two model calibration criteria, RMSE and Nash–Sutcliffe model efficiency (NSME) (Nash and Sutcliffe, 1970), were used to evaluate the simulation results:

$$\mathrm{RMSE}=\sqrt{\frac{\sum_{i=1}^{n}\left(O_i-P_i\right)^2}{n}} \qquad [12]$$

$$\mathrm{NSME}=1.0-\frac{\sum_{i=1}^{n}\left(O_i-P_i\right)^2}{\sum_{i=1}^{n}\left(O_i-O_{\mathrm{avg}}\right)^2} \qquad [13]$$

where P_i is the ith predicted value, O_i is the ith observed value, O_{avg} is the average of the observed or simulated values, and n is the number of data pairs. A paired t-test was used for statistical significance testing of the differences between these methods across the four sites.

RESULTS AND DISCUSSION

Model calibration and evaluation (cross-validation) were performed at four sites (C1, C2, D1, and E2) in an agricultural field at the Drake Farm (Fig. 1). It is not feasible to show detailed results at all four sites, so we focus here on Site E2. This site contained the most data vertically (10 depths) and temporally (no missing data for the periods analyzed). The following results apply to Site E2 unless otherwise noted.

Initial PEST Simulation Results

The default parameters based on soil survey data and soil class in RZWQM2 resulted in high RMSE values (0.078 $m^3\ m^{-3}$ for 2002 and 0.080 $m^3\ m^{-3}$ for 2004) and negative NSME values (−0.16 for 2002 and −0.19 for 2004). These simulation results

Table 2. Site E2 statistical results of the measured soil water content (SWC) at each depth during the 2002–2003 and 2004–2005 fallow periods.

Depth	Soil water content									
	Fallow 1 (2002–2003)					Fallow 2 (2004–2005)				
	Min.	Max.	Mean	SD	ΔSWC†	Min.	Max.	Mean	SD	ΔSWS
cm	$m^3\ m^{-3}$									
30	0.15	0.40	0.29	0.11	0.21	0.22	0.42	0.32	0.07	0.13
40	0.18	0.40	0.30	0.10	0.17	0.21	0.43	0.30	0.08	0.13
50	0.18	0.39	0.28	0.09	0.17	0.19	0.43	0.28	0.08	0.13
60	0.14	0.35	0.24	0.09	0.16	0.16	0.39	0.24	0.08	0.13
70	0.14	0.34	0.22	0.09	0.16	0.15	0.39	0.24	0.09	0.15
80	0.15	0.33	0.22	0.07	0.15	0.16	0.39	0.24	0.09	0.15
90	0.12	0.24	0.16	0.05	0.11	0.13	0.34	0.20	0.09	0.14
120	0.10	0.15	0.12	0.02	0.03	0.12	0.31	0.18	0.08	0.15
150	0.12	0.16	0.13	0.02	0.03	0.13	0.28	0.18	0.06	0.12
170	0.13	0.17	0.15	0.01	0.03	0.15	0.26	0.18	0.04	0.09

† ΔSWC is the difference in soil water content at each depth between the beginning and end of the period.

were significantly improved by the initial optimization results using PEST based on the survey data as presented in Fig. 2 and 3. In general, simulated and measured soil water contents at different depths showed similar trends, with better calibration results than cross-validation results. Large differences in model performance were found among these methods (Fig. 3), and the SWRC1K$_{in}$ and SWRCλK$_{in}$ methods generally produced better simulation results than the other methods. Abnormal soil evaporation occurred for the two-parameter methods (SWRC2K$_{in}$ and SWRC2K$_{es}$), however, with simulated annual soil evaporation values of <6 cm (only about 18% of rainfall) associated with unreasonable combinations of the soil hydraulic parameters $\theta_{1/3}$, θ_{15}, θ_s and K_{sat} (Table 3), which is obviously lower than the observed data on bare soil from other studies under similar climate conditions (Burt et al., 2005).

These results confirm that PEST optimization can be sensitive to the initial parameter values and ranges and may result in poor calibration results, especially when parameter values are not well constrained (Doherty, 2004). Some calibrated parameter values (θ_s) also reached the upper or lower limits for the soil type, probably also due to the limited data available, parameter constraints, and model error during the optimizations. As reported from some other studies (Skahill and Doherty, 2006), the sensitivity of PEST to local minima may result in abnormal calibrated parameters. The initial values and boundary conditions selected based on prior information and other methods proved useful for more effective parameter estimation to simulate soil water processes, as illustrated by other studies (Mertens et al., 2005; Kuzmin et al., 2008).

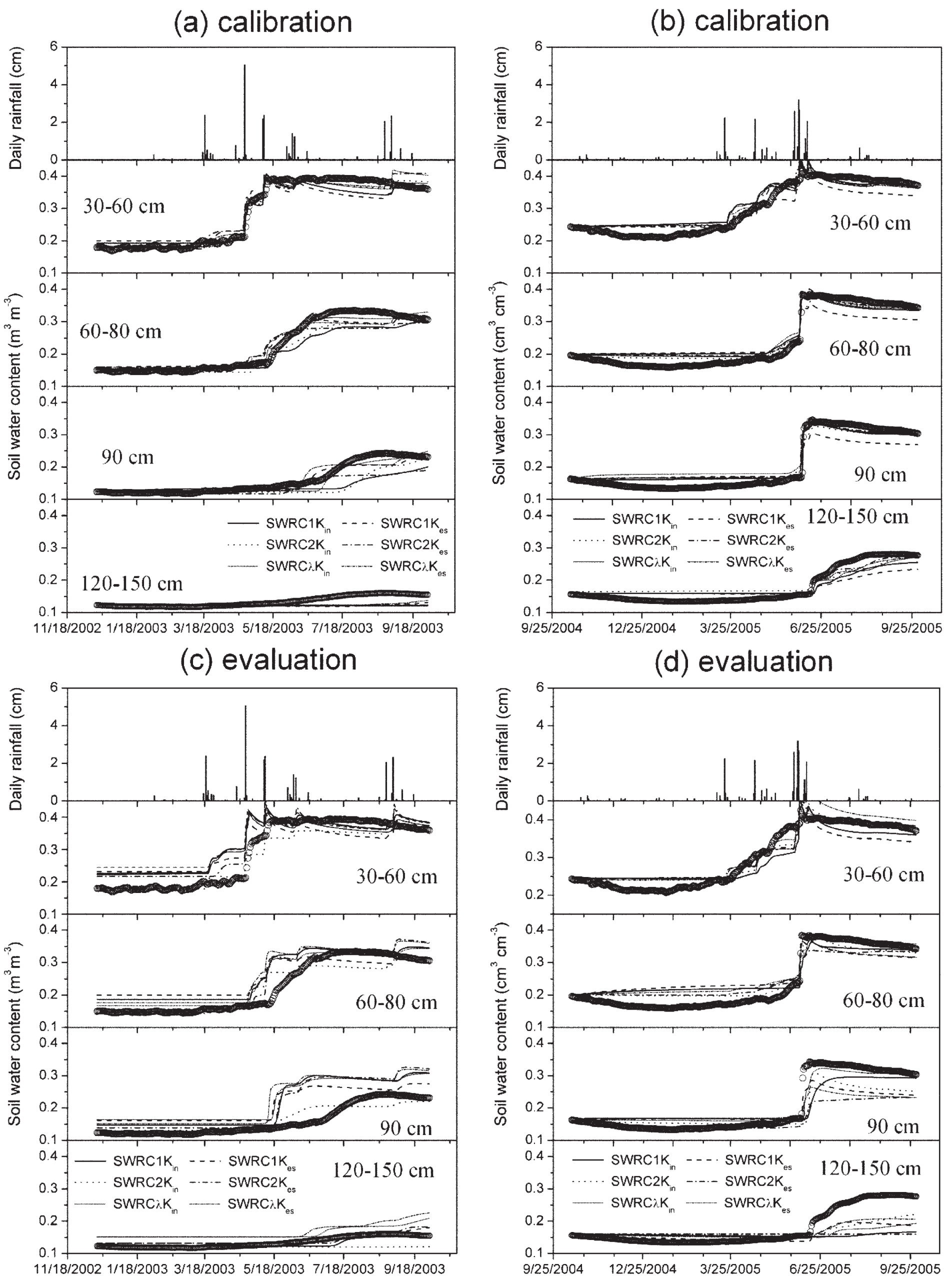

Fig. 2. Comparisons of observed and simulated soil water content at Site E2 in each layer for the six parameter estimation methods using PEST: 2002–2003 fallow for (a) calibration or (c) evaluation, and 2004–2005 fallow for (b) calibration and (d) evaluation. Soil water contents were averaged from 30-, 40-, and 50-cm depths, 60-, 70-, and 80-cm depths, 90-cm depth, and 120-, 150-, and 170-cm depths for the simulated and measured data. The SWRC1K$_{in}$ and SWRC1K$_{es}$ are one-parameter methods, SWRC2K$_{in}$ and SWRC2K$_{es}$ are two-parameter methods, and SWRCλK$_{in}$ and SWRCλK$_{es}$ are full Brooks–Corey methods.

Latin Hypercube Sampling Results

Latin hypercube sampling was used to sample parameter combinations and to search the full physical ranges of these soil hydraulic parameters in RZWQM2. The first search boundaries were based on soil type for the one-parameter estimation methods. The parameter ranges for θ_s, θ_r, $\theta_{1/3}$, and K_{sat} at each soil layer were 0.43 to 0.55 m^3 m^{-3}, 0.01 to 0.05 m^3 m^{-3}, 0.1 to 0.4 m^3 m^{-3}, and 0.01 to 10 cm h^{-1}, respectively, except for the surface layer, where θ_s and K_{sat} were constrained to 0.46 to 0.62 m^3 m^{-3} and 0.5 to 15 cm h^{-1}, respectively. The values of θ_s in the surface layer (0–15 cm) were relatively high due to surface tillage. Note that the parameter values of the tilled layer represent the consolidated (lowest) values; these are modified (increased) by tillage in RZWQM2 and reduced again by reconsolidation after rainfall.

For the two-parameter methods (SWRC2K$_{in}$ and SWRC2K$_{es}$), unreasonable combinations of θ_{15} and $\theta_{1/3}$ occurred when sampling the two parameters using the LHS method. Instead, we sampled the parameters θ_s, K_{sat}, λ, and ψ_b for the full BC method (SWRCλK$_{in}$ and SWRCλK$_{es}$) based on soil type for each layer in RZWQM2, then calculated θ_{15} and $\theta_{1/3}$ using Eq. [7] and [8] for the two-parameter methods. The distributions and relationships among these parameters showed similar trends between the one-parameter method and the full BC method. The deviations in estimated values of K_{sat} and θ_{15} from $\theta_{1/3}$ were mainly due to the variations in θ_s and θ_r. The relationship between $\theta_{1/3}$ and θ_{15} for SWRCλK$_{es}$ showed a linear correlation, with a larger deviation than for the SWRC1K$_{in}$ method.

Profile soil water balance is simulated by RZWQM2, whereas a full water balance is not available from water content measurements at discrete depths. Because the soil water contents in the surface layer (0–15 cm) were not measured, it was difficult to refine the soil hydraulic parameters in this layer. Soil hydraulic properties in the surface layer, however, control water flux across the land surface and soil water content in the deeper layers. Soil evaporation and runoff control the water balance under fallow conditions. For example, overestimation of soil evaporation in the model results in less water available for deep percolation.

The relationship between soil water storage below the surface layer and soil hydraulic parameters in the surface layer were quantified to refine the ranges of these soil hydraulic parameters in the layer. As an example, for the SWRC1K$_{in}$ method, soil evaporation and soil water storage during the fallow period from 2004 to 2005 responded in opposite directions to the changes in $\theta_{1/3}$ and K_{sat}. The estimated values of soil water storage change during the fallow period based on the measured water content data (Table 2) were about 14 to 16 cm, and the reasonable ranges of $\theta_{1/3}$ should fall within 0.10 to 0.25 m^3 m^{-3}. In same way, the range in K_{sat} can be estimated to be 0.5 to 10 cm h^{-1}. This range in K_{sat} is consistent with the measured values at the surface based on steady, ponded infiltration (Green et al., 2009).

Scatter plots of model performance (RMSE) vs. individual parameters (Fig. 4) were used to identify the model response to these parameters at each layer and to refine the ranges of these parameters in all layers. Figure 4 shows some examples of the sensitivity of simulated water content at the 30-cm depth to soil hydraulic parameters using different methods. Values of $\theta_{1/3}$ were computed from the full BC parameters for comparison with the one-parameter methods. The optimal range of $\theta_{1/3}$ was well-defined for all estimation methods (Fig. 4a, 4b, 4d, and 4e), as were the optimal ranges of K_{sat} for the constrained parameter methods of SWRC1K$_{es}$ and SWRCλK$_{es}$ (Fig. 4g and 4h) and the optimal range of the pore size distribution parameter λ for SWRCλK$_{in}$ (Fig. 4f). No obvious relationship between model performance and ψ_b was found (Fig. 4c), however. No obvious relationship between model performance and K_{sat} was found for the SWRCλK$_{in}$ method (Fig. 4i), indicating less parameter correlation than assumed using SWRCλK$_{es}$ (Fig. 4h). Unconstrained parameter interactions within the K$_{in}$ methods make the optimal K_{sat} value less well-defined (non-unique), but the minimum values of the RMSE are similar among the methods. Optimal parameter values from PEST, for example, $\theta_{1/3}$ and θ_{15} were highly correlated with θ_s, with correlation coefficient values of 0.5 to 0.8 for some soil depths.

The best parameter combinations and reasonable ranges of these parameters with best model performance for the two fallow periods were selected for further optimization by PEST based on 6000 simulation runs. As indicated in Fig. 4, there are many parameter sets that produced similar simulation results for the two fallow periods. The ranges of these parameters selected by the LHS method were slightly different among the six methods in RZWQM2. The best simulation results based on 6000 simulation runs sampled by LHS are presented in Fig. 5 and Table 4. For the two fallow periods, a slightly better model performance, with lower RMSE and higher NSME values, occurred for the 2004–2005 fallow period than for the 2002–2003 fallow period. The model generally overpredicted soil water content during the winter and underpredicted soil water content during summer. The one-parameter methods produced better simulation results (high NSME values) for the two fallow periods than SWRCλK$_{in}$, but similar to SWRCλK$_{es}$ (Fig. 5).

In theory, the full BC method is more flexible in regulating the combination of these parameters than the one-parameter method, but the search space increases exponentially to the power of the number of independent parameters explored. Under the current condition with 6000 simulation runs for

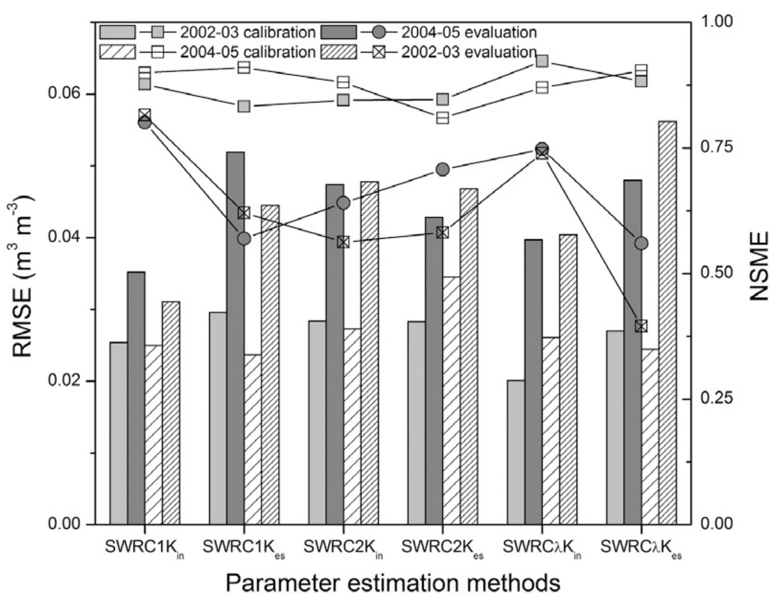

Fig. 3. Comparisons of the model performances for reproducing the measured soil water contents at Site E2 by the six parameter estimation methods in RZWQM2 using PEST with different temporally measured soil water data. The RMSE (bars) and Nash–Sutcliffe model efficiency (NSME) (points) were calculated from all the measured and simulated data averaged across all the depths. The SWRC1K$_{in}$ and SWRC1K$_{es}$ are one-parameter methods, SWRC2K$_{in}$ and SWRC2K$_{es}$ are two-parameter methods, and SWRCλK$_{in}$ and SWRCλK$_{es}$ are full Brooks–Corey methods.

Table 3. Calibrated soil hydraulic parameters of soil water content at 33 kPa and 1500 kPa ($\theta_{1/3}$ and θ_{15}) and saturated hydraulic conductivity (K_{sat},) at each depth for the six parameter estimation methods (Table 1) at Site E2 using Latin hypercube sampling (LHS), the PEST parameter estimation program, or LHS and PEST combined.

Method and data set	Depth	SWRC1K$_{in}$			SWRC1K$_{es}$			SWRC2K$_{in}$			SWRC2K$_{es}$			SWRCλK$_{in}$			SWRCλK$_{es}$		
		$\theta_{1/3}$	θ_{15}	K_{sat}	$\theta_{1/3}$	θ_{15}	K_{sat}	$\theta_{1/3}$	θ_{15}	K_{sat}	$\theta_{1/3}$	θ_{15}	K_{sat}	$\theta_{1/3}$	θ_{15}	K_{sat}	$\theta_{1/3}$	θ_{15}	K_{sat}
	cm	– m^3 m^{-3} –		cm h^{-1}	– m^3 m^{-3} –		cm h^{-1}	– m^3 m^{-3} –		cm h^{-1}	– m^3 m^{-3} –		cm h^{-1}	– m^3 m^{-3} –		cm h^{-1}	– m^3 m^{-3} –		cm h^{-1}
PEST	0–15	0.23	0.11	1.40	0.35	0.24	4.65	0.23	0.14	1.69	0.26	0.19	1.08	0.20	0.13	1.01	0.28	0.18	10.41
2002–2003	15–55	0.31	0.19	0.95	0.32	0.20	2.54	0.30	0.16	1.10	0.35	0.14	1.59	0.32	0.18	0.68	0.37	0.18	0.76
calibration	55–85	0.27	0.15	1.72	0.28	0.16	4.22	0.23	0.12	1.34	0.25	0.13	3.48	0.27	0.16	0.60	0.29	0.16	3.23
	85–105	0.20	0.10	1.41	0.20	0.10	11.35	0.17	0.08	1.21	0.16	0.08	16.72	0.18	0.07	1.14	0.21	0.12	1.99
	105–170	0.10	0.03	0.59	0.14	0.07	19.47	0.18	0.08	1.05	0.15	0.11	5.00	0.10	0.04	0.60	0.18	0.08	3.43
PEST	0–15	0.10	0.04	1.29	0.35	0.24	3.82	0.10	0.04	1.57	0.17	0.10	27.85	0.09	0.05	1.12	0.18	0.12	25.74
2004–2005	15–55	0.34	0.23	1.17	0.35	0.23	0.82	0.35	0.21	0.50	0.32	0.22	2.39	0.35	0.22	0.85	0.36	0.24	1.07
calibration	55–85	0.31	0.19	1.29	0.32	0.20	0.18	0.32	0.15	1.80	0.28	0.16	4.30	0.32	0.17	1.43	0.33	0.18	1.49
	85–105	0.27	0.15	1.32	0.28	0.16	0.47	0.28	0.14	10.00	0.24	0.14	1.16	0.28	0.16	1.39	0.28	0.15	2.28
	105–170	0.24	0.12	1.31	0.25	0.13	0.92	0.27	0.16	0.52	0.22	0.13	1.84	0.26	0.15	1.19	0.26	0.15	1.08
LHS	0–15	0.19	0.08	7.13	0.19	0.08	19.78							0.15	0.06	6.03	0.15	0.06	15.35
	15–55	0.35	0.23	3.87	0.35	0.23	0.56							0.33	0.20	5.28	0.33	0.20	1.60
	55–85	0.29	0.17	1.31	0.29	0.17	1.21							0.29	0.13	5.07	0.29	0.13	2.46
	85–105	0.23	0.12	4.81	0.23	0.12	5.36							0.22	0.07	5.41	0.22	0.07	4.75
	105–170	0.22	0.11	3.68	0.22	0.11	6.47							0.16	0.07	4.83	0.16	0.07	1.46
LHS+PEST	0–15	0.22	0.10	3.25	0.22	0.10	16.65	0.27	0.14	5.28	0.22	0.13	16.45	0.09	0.05	0.62	0.21	0.12	13.03
2002–2003	15–55	0.32	0.20	0.22	0.33	0.21	1.46	0.39	0.15	1.44	0.31	0.17	0.75	0.33	0.17	0.08	0.36	0.18	0.95
calibration	55–85	0.27	0.15	1.31	0.29	0.16	2.58	0.31	0.13	6.24	0.26	0.15	5.21	0.31	0.17	0.10	0.28	0.13	3.75
	85–105	0.17	0.07	0.77	0.20	0.10	9.72	0.22	0.13	2.92	0.20	0.10	8.12	0.23	0.11	5.59	0.19	0.08	5.49
	105–170	0.15	0.07	0.50	0.15	0.08	18.25	0.27	0.08	3.62	0.27	0.07	1.83	0.15	0.07	2.20	0.15	0.07	9.53
LHS+PEST	0–15	0.15	0.07	3.25	0.15	0.07	30.33	0.19	0.12	8.00	0.20	0.13	18.39	0.12	0.07	2.71	0.14	0.08	35.64
2004–2005	15–55	0.34	0.22	0.53	0.36	0.24	0.23	0.30	0.15	0.17	0.34	0.23	1.25	0.37	0.22	0.14	0.37	0.24	0.84
calibration	55–85	0.30	0.17	1.12	0.32	0.19	0.57	0.24	0.10	0.89	0.30	0.16	2.13	0.35	0.16	0.91	0.34	0.17	0.52
	85–105	0.25	0.13	1.12	0.25	0.13	5.67	0.21	0.10	2.90	0.26	0.14	2.11	0.30	0.14	2.71	0.30	0.14	1.06
	105–170	0.24	0.12	3.44	0.23	0.12	4.79	0.20	0.11	5.20	0.24	0.14	3.02	0.28	0.15	4.03	0.27	0.15	1.95

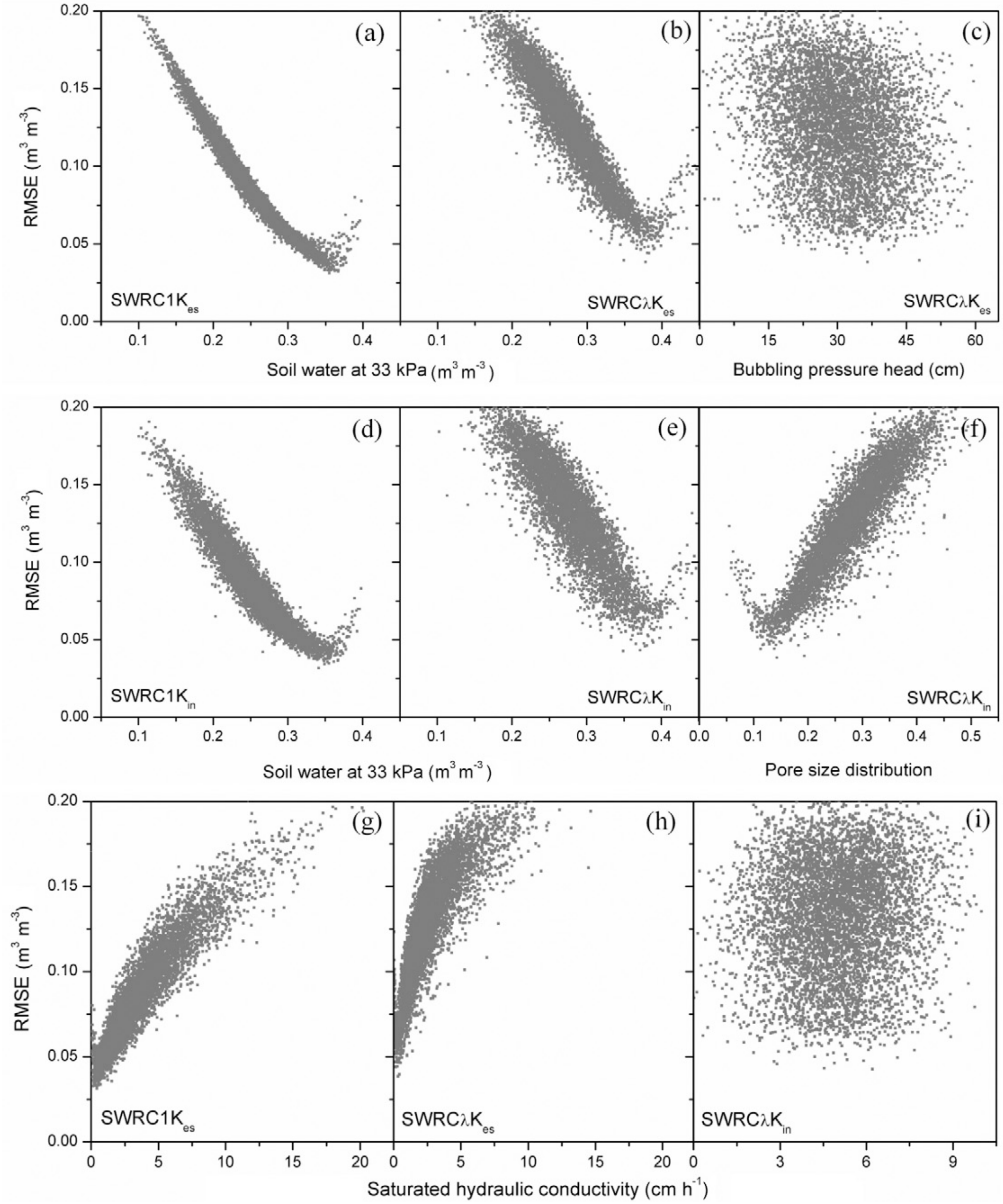

Fig. 4. Errors in simulated soil water content at Site E2 at the 30-cm depth vs. soil water content at 33 kPa, bubbling-pressure suction, pore-size distribution parameter λ, and saturated hydraulic conductivity for the parameter estimation methods (2004–2005 fallow period) based on Latin hypercube sampling search analysis (6000 simulation runs). The SWRC1K$_{in}$ and SWRC1K$_{es}$ are one-parameter methods and SWRCλK$_{in}$ and SWRCλK$_{es}$ are full Brooks–Corey methods.

each method, the above results indicated that the one-parameter method in RZWQM2 can be more efficient than the two-parameter method. Reducing simulation runs by using the relationships between parameters (Eq. [7–9]) is a useful and efficient way to search and refine the soil hydraulic parameters in RZWQM2, given limited computational power where each set of 6000 runs took more than 12 h on a desktop computer.

The estimated value of K_{sat} differed between SWRC1K$_{in}$ and SWRC1K$_{es}$ and between SWRCλK$_{in}$ and SWRCλK$_{es}$, but showed similar trends with soil depth (Table 3). Across the six methods, the selected parameter values of $\theta_{1/3}$ and θ_{15} generally increased from the surface layer to the second and third layers and decreased in the last two layers. In general, K_{sat} values changed inversely with $\theta_{1/3}$ (per Eq. [10]) and were obviously higher for the SWRC1K$_{es}$ and SWRCλK$_{es}$ methods than for the SWRC1K$_{in}$ and SWRCλK$_{in}$ methods in the surface layer, becoming closer at the deeper layers.

Latin Hypercube Sampling plus PEST Optimization Results

For the six methods in RZWQM2, better calibration results were obtained than evaluation results for LHS + PEST optimizations, and overpredicted soil water contents generally occurred during the winter seasons, while underpredicted soil water contents occurred during the summer and autumn (Fig. 6; Table 4). The magnitude of change in seasonal water contents

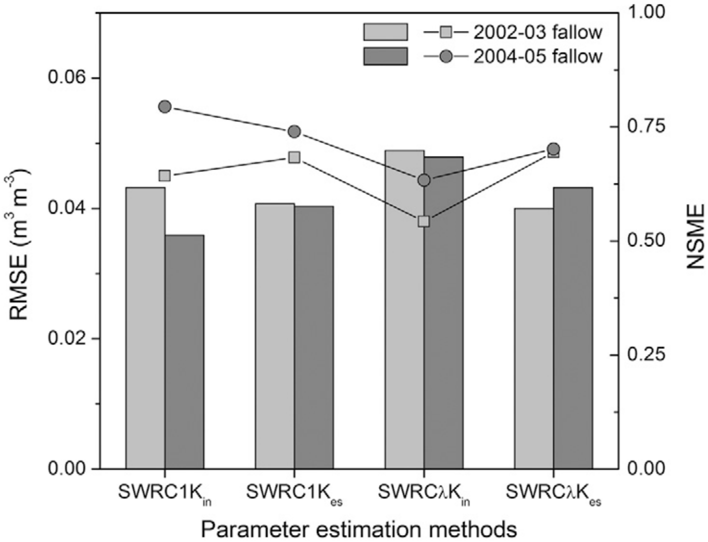

Fig. 5. Comparisons of the model performances at Site E2 for four parameter estimation methods in RZWQM2 using Latin hypercube sampling. The RMSE (bars) and Nash-Sutcliffe model efficiency (NSME) (points) were calculated from all the measured and simulated data at all soil depths. The SWRC1K$_{in}$ and SWRC1K$_{es}$ are one-parameter methods and SWRCλK$_{in}$ and SWRCλK$_{es}$ are full Brooks–Corey methods.

was generally simulated well, but the timing of the main wetting front was not always reproduced, particularly for the evaluation period (e.g., Site E2 evaluation for 2002–2003 shown in Fig. 6c). Measured water contents were also more temporally stable than simulated values.

The temporal data sets (the two fallow periods) used for calibrations and cross-validation influenced the simulation results. When using 2002–2003 data for calibration, the soil water content was generally overpredicted during the evaluation period, although there were underpredictions in soil water during the summer (Fig. 6a and 6d); using 2004–2005 data for calibration, soil water was overpredicted during both calibration and evaluation (Fig. 6b and 6c). This result is similar to the simulation results from our initial PEST optimizations (Table 4). Methods SWRC1K$_{es}$ and SWRCλK$_{es}$ produced worse model performance than the other methods when using 2004–2005 fallow data for calibration, and the six parameter methods produced similar model performance when 2002–2003 fallow data were used (Table 4).

Similar trends in NSME with soil depth were found across the six parameter estimation methods, where lower NSME values generally occurred at the deepest layers (Table 4). The negative NSME values at the deepest depth for all the methods indicated a worse model performance at this layer than at other layers. This result was probably due to the small variance in the measured values causing low NSME values even if the RMSE values are not large (see Eq. [12] and [13]).

The optimized parameter values using LHS + PEST showed similar trends with depth among the six methods or the two data sets used for calibration (Table 3). When using 2002–2003 fallow data for calibration, calibrated parameters of $\theta_{1/3}$, θ_{15} and K_{sat} for SWRC1K$_{in}$ were generally lower than for the other methods; using 2004–2005 fallow data for calibration, these parameters for SWRC2K$_{in}$ were relatively lower than the other methods except for in the surface layer. The resulting water retention characteristics and hydraulic conductivity curves for SWRC1K$_{in}$ (as an example) are illustrated for each calibration period and soil layer in Fig. 7. Higher values of K_{sat} in the surface layer were obtained for the first calibration period (2002–2003) than for the second calibration period (2004–2005), along with changes in the SWRC. These different soil hydraulic properties result in different soil evaporation and soil water redistribution to deeper layers. Comparing these parameters in the deep layer (85–170 cm), different results were found between the two calibration periods. As shown in Fig. 2 and 8, the underpredicted soil water contents in the deep layer (2004–2005 fallow period) were mainly caused by higher soil evaporation. In Fig. 3 and 9, the overpredicted soil water contents in these deep layers (2002–2003 fallow period) were mainly caused by lower soil evaporation and less drainage from the soil profile.

Wagener et al. (2003) showed that optimal model parameter sets can change with time, with variable degrees of "identifiability" depending on the system states and boundary conditions. Therefore, we were not surprised that the cross-validation results were poorer than calibration of either time period. For example, differences between simulated and measured soil water at 90 cm may highlight the need for improved evaporation modeling and possible limitations of the model structure in terms of the fixed depths of soil horizons.

In general, the SWRC1K$_{in}$ and SWRC2K$_{in}$ methods produced better simulation results during the cross-validations than the other methods. The relatively large deviations between measured and simulated soil moisture for the 60- to 90-cm layers were probably caused by unreasonable soil hydraulic parameters in the surface layer (0–15 cm), and water content was not measured in the surface horizon. More reasonable soil parameters in the surface layer can improve soil evaporation and other components of the soil water balance simulation and result in better soil moisture simulations in deeper layers. Comparing the measured and simulated data across seasons, the simulated soil moisture generally showed quicker responses to rainfall events and soil evaporation than the measured data (Fig. 2, 3, 8, and 9). Several factors can contribute to this result, such as rainfall patterns for the two fallow periods, soil hydraulic property variations across depths, and agronomic management effects (e.g., tillage) on soil properties. Soil hydraulic property variations across depths should be a main reason because soil horizon depths were delineated based on an Order 2 soil survey for the site, which may not accurately represent the specific soil horizon depths at each probe location. Furthermore, the assumption of uniform soil properties for each layer in the model may not accurately represent the real field conditions, where fine-scale soil layering affects the horizon-scale average hydraulic properties in nonlinear ways (e.g., Green et al., 1996).

Table 4. The model calibration criteria of RMSE and Nash–Sutcliffe model efficiency (NSME) for simulated soil water content at each individual layer for the six parameter estimation methods (Table 1) at Site E2.

Data set	Depth	SWRC1K$_{in}$		SWRC1K$_{es}$		SWRC2K$_{in}$		SWRC2K$_{es}$		SWRCλK$_{in}$		SWRCλK$_{es}$	
		RMSE	NSME	RMSE	NSME	RMSE	NSME	RMSE	NSME	RMSE	NSME	RMSE	NSME
	cm	$m^3 m^{-3}$		$m^3 m^{-3}$		$m^3 m^{-3}$		$m^3 m^{-3}$		$m^3 m^{-3}$		$m^3 m^{-3}$	
						PEST parameter estimation program							
2002–2003 calibration	30	0.028	0.91	0.044	0.80	0.026	0.93	0.031	0.90	0.022	0.95	0.028	0.92
	60	0.015	0.97	0.032	0.85	0.026	0.90	0.035	0.82	0.016	0.96	0.029	0.87
	90	0.013	0.93	0.018	0.86	0.028	0.63	0.023	0.76	0.013	0.93	0.017	0.87
	150	0.022	−1.09	0.023	−1.24	0.02	−0.50	0.019	−0.43	0.022	−1.08	0.021	−0.96
2004–2005 evaluation	30	0.021	0.93	0.034	0.82	0.034	0.80	0.048	0.64	0.028	0.87	0.027	0.89
	60	0.039	0.81	0.049	0.71	0.038	0.83	0.034	0.86	0.024	0.93	0.023	0.94
	90	0.033	0.86	0.049	0.67	0.052	0.63	0.027	0.91	0.031	0.87	0.024	0.92
	150	0.056	−0.02	0.057	0.03	0.062	−0.12	0.062	−0.12	0.026	0.78	0.021	0.88
2004–2005 calibration	30	0.028	0.88	0.04	0.75	0.025	0.90	0.026	0.89	0.026	0.89	0.033	0.82
	60	0.027	0.91	0.039	0.81	0.025	0.93	0.022	0.94	0.036	0.84	0.039	0.82
	90	0.022	0.94	0.033	0.86	0.023	0.93	0.025	0.91	0.025	0.92	0.053	0.61
	150	0.037	0.59	0.024	0.85	0.019	0.90	0.02	0.89	0.053	0.06	0.040	0.57
2002–2003 evaluation	30	0.038	0.85	0.065	0.57	0.036	0.87	0.044	0.80	0.050	0.74	0.059	0.64
	60	0.026	0.89	0.06	0.45	0.038	0.75	0.039	0.76	0.041	0.74	0.052	0.56
	90	0.04	0.28	0.07	−1.21	0.064	−0.89	0.062	−0.75	0.069	−1.19	0.075	−1.55
	150	0.039	−4.98	0.036	−5.44	0.024	−1.43	0.033	−3.62	0.037	−5.72	0.042	−7.55
						Latin hypercube sampling							
2002–2003	30	0.053	0.71	0.054	0.70					0.061	0.62	0.05	0.74
	60	0.046	0.68	0.041	0.75					0.054	0.56	0.041	0.74
	90	0.041	0.24	0.028	0.65					0.045	0.08	0.044	0.12
	150	0.026	−1.84	0.023	−1.22					0.025	−1.81	0.021	−0.94
2004–2005	30	0.034	0.81	0.039	0.76					0.046	0.66	0.047	0.65
	60	0.038	0.82	0.044	0.76					0.052	0.68	0.047	0.74
	90	0.037	0.82	0.045	0.72					0.051	0.65	0.032	0.87
	150	0.032	0.70	0.032	0.72					0.042	0.50	0.035	0.65
						Latin hypercube sampling + PEST							
2002–2003 calibration	30	0.035	0.87	0.046	0.78	0.033	0.88	0.028	0.92	0.026	0.93	0.025	0.90
	60	0.024	0.92	0.035	0.82	0.037	0.79	0.027	0.89	0.020	0.94	0.021	0.95
	90	0.029	0.61	0.02	0.82	0.022	0.79	0.017	0.86	0.013	0.92	0.025	0.91
	150	0.022	−0.99	0.022	−1.00	0.023	−1.25	0.017	−0.36	0.022	−1.06	0.021	0.88
2004–2005 evaluation	30	0.028	0.87	0.036	0.80	0.035	0.80	0.028	0.87	0.022	0.93	0.047	0.77
	60	0.031	0.88	0.048	0.72	0.027	0.91	0.044	0.77	0.044	0.76	0.034	0.82
	90	0.028	0.87	0.036	0.80	0.035	0.80	0.028	0.87	0.041	0.77	0.057	−0.50
	150	0.042	0.57	0.05	0.54	0.049	0.43	0.047	0.62	0.051	0.16	0.038	−6.40
2004–2005 calibration	30	0.026	0.90	0.032	0.84	0.026	0.89	0.026	0.89	0.030	0.91	0.029	0.86
	60	0.028	0.90	0.036	0.84	0.019	0.95	0.022	0.94	0.035	0.81	0.023	0.94
	90	0.024	0.92	0.035	0.84	0.024	0.92	0.024	0.92	0.023	0.75	0.023	0.93
	150	0.030	0.76	0.031	0.74	0.022	0.85	0.020	0.88	0.018	−0.55	0.022	0.87
2002–2003 evaluation	30	0.045	0.79	0.062	0.60	0.032	0.90	0.050	0.73	0.041	0.73	0.061	0.61
	60	0.041	0.73	0.058	0.48	0.029	0.87	0.045	0.67	0.043	0.77	0.048	0.64
	90	0.055	−0.36	0.050	−0.14	0.046	0.05	0.073	−1.42	0.053	0.63	0.073	−1.44
	150	0.024	−1.40	0.029	−2.50	0.028	−2.32	0.036	−5.90	0.048	0.29	0.045	−8.96

Comparisons of Calibration Procedures, Methods, and Data Sets

Both PEST and LHS + PEST improved the model performance significantly in all cases compared with the simulation results using the default parameter values (Fig. 8). The simulation results from the LHS method were more stable between the two fallow data sets than the PEST optimizations but with higher RMSE values (Table 5). Although better calibration results were obtained from the PEST procedure than the LHS procedure, unrealistic soil evaporation with abnormal calibrated parameters occurred, as discussed above. Similar results also occurred when the same calibration procedure was applied to the other three sites, where worse simulation results were generally obtained than the model performance at Site E2 (Table 5). The selected initial values and ranges of these parameters from LHS avoided this problem and resulted in similar or better simulation results (lower RMSE and higher NSME values) using PEST in subsequent optimizations across the other three sites (Table 5; Fig. 8). The worst simulation result for the different methods occurred at Site D1, with low or negative NSME values for PEST

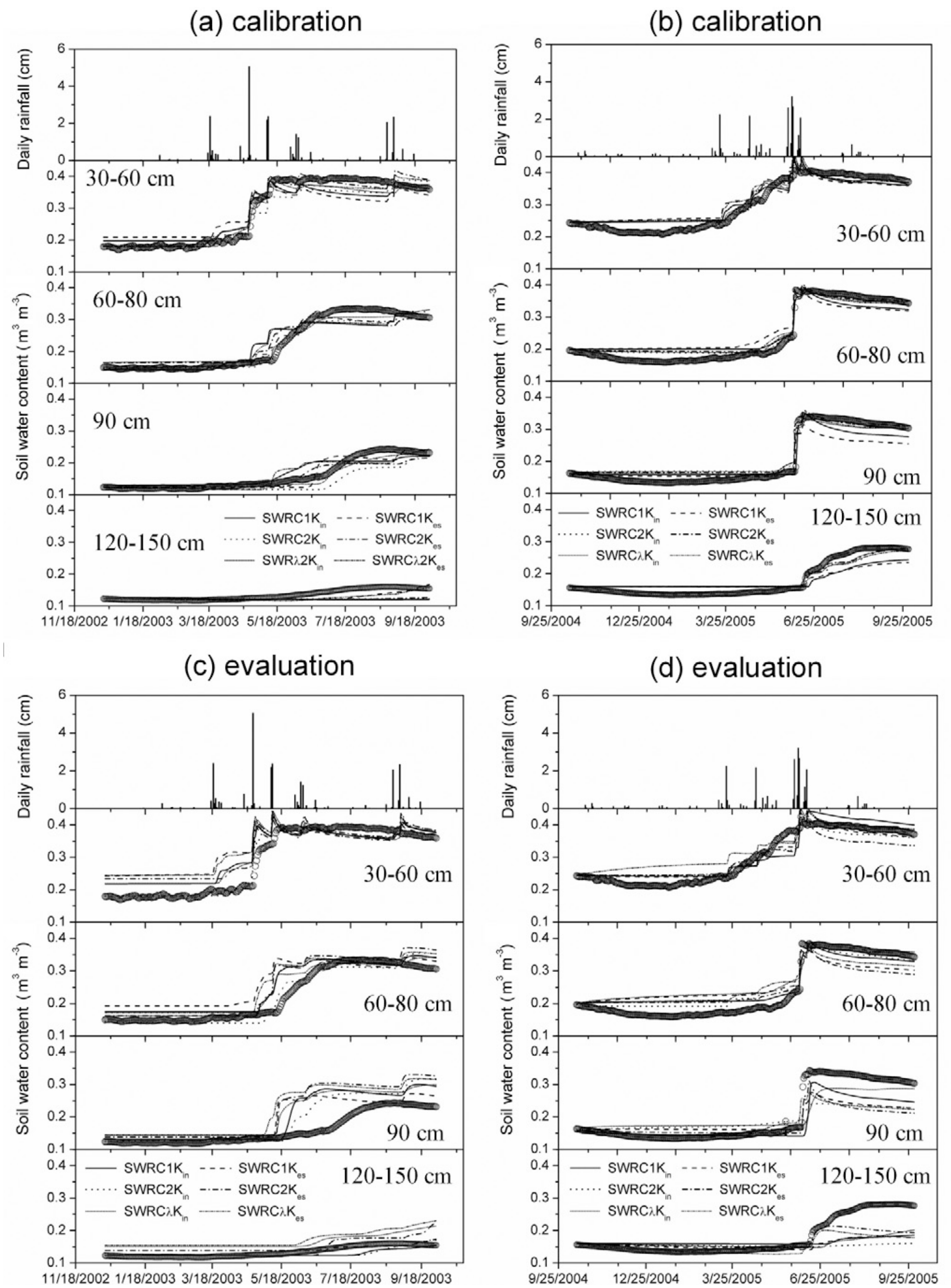

Fig. 6. Comparisons of observed and simulated soil water content at Site E2 in each layer for the six parameter estimation methods using the Latin hypercube sampling (LHS) + PEST procedure: 2002–2003 fallow for (a) calibration or (c) evaluation, and 2004–2005 fallow for (b) calibration and (d) evaluation. Soil water contents were averaged from 30-, 40-, and 50-cm depths, 60-, 70-, and 80-cm depths, 90-cm depth, and 120-, 150-, and 170-cm depths for simulated and measured data. The SWRC1K$_{in}$ and SWRC1K$_{es}$ are one-parameter methods, SWRC2K$_{in}$ and SWRC2K$_{es}$ are two-parameter methods, and SWRCλK$_{in}$ and SWRCλK$_{es}$ are full Brooks–Corey methods.

optimization. For Sites C1 and C2, the relative RMSE (RMSE/measured mean) was about 30% for the whole simulation period. The greatest differences between measured and simulated soil water contents occurred mainly during winter in the deeper layers and were similar to the simulation errors at Site E2.

Although the simulation results for Sites C1, C2, and D1 were worse than for Site E2, simulated soil water contents improved going from the initial PEST procedure to the LHS + PEST calibration procedure, suggesting an advantage in calibrating soil hydraulic parameters in RZWQM2 by combining the LHS and PEST methods (Table 5). The better PEST calibrations with worse cross-validation results compared with LHS + PEST optimization across the three sites indicate an overcalibration for the initial PEST calibrations. The initial values and ranges of soil hydraulic parameters from LHS search selections helped PEST optimization to obtain more physically realistic combinations of these parameters but at the expense of increased computing time because about 200 to 400 runs were used by the PEST optimization procedure. By selecting only the initial values and ranges of these parameters by LHS, the model runs can be reduced dramatically. Across the four sites, the SWRC1K$_{in}$ method generally resulted in better simulation results for the initial PEST optimization or LHS search analysis procedure compared with the other parameter estimation methods. For the LHS + PEST optimizations, similar simulation results were obtained across the different methods in RZWQM2.

The performance of these methods varied depending on the specific calibration procedures and probe locations (data sets) (Fig. 8; Table 5). For example, at Site E2, the one-parameter methods performed better than the two-parameter methods when using the LHS analysis, while better simulation results were obtained with the two-parameter methods than the one-parameter methods using the LHS + PEST procedure. Similar results occurred at Site D1, while the SWRC2K$_{in}$ method resulted in better simulations at Site C1 compared with the other methods. On the other hand, all methods produced similar simulation results at Site C2. Based on these results and a previous study by Ma et al. (2009), different soil hydraulic parameter estimation methods should be evaluated for specific studies, and we cannot identify one method that works best in all cases.

The parameters calibrated by the LHS + PEST procedure for the six methods are presented in Table 3. Similar trends in $\theta_{1/3}$, θ_{15}, and K_{sat} occurred with soil depth among the parameter estimation methods, but large differences in K_{sat} were found between the two different methods of estimating K_{sat} (denoted K_{in} and K_{es}). Across the six methods, no significant differences in the values of θ_s, $\theta_{1/3}$, and θ_{15} were found (P = 0.274, where P is the probability value for significance testing according to a paired t-test). These results suggested that the calibrated parameter values at Site E2 were relatively stable among the six methods; however, strong interactions between these soil hydraulic parameters resulted in different model performance. Comparing the calibrated $\theta_{1/3}$ and θ_{15} values from the two data sets across these different methods, lower values in the surface layer (0–15 cm) and higher values in the deeper layers (15–105 cm) were found in most cases when the calibration data from 2004–2005 were used compared with 2002–2003 (Table 3). This result shows the uncertainty in calibrating soil hydraulic parameters associated with different temporal patterns in the measured data. This also confirms the necessity of cross-validation, as done here, for model parameter evaluation.

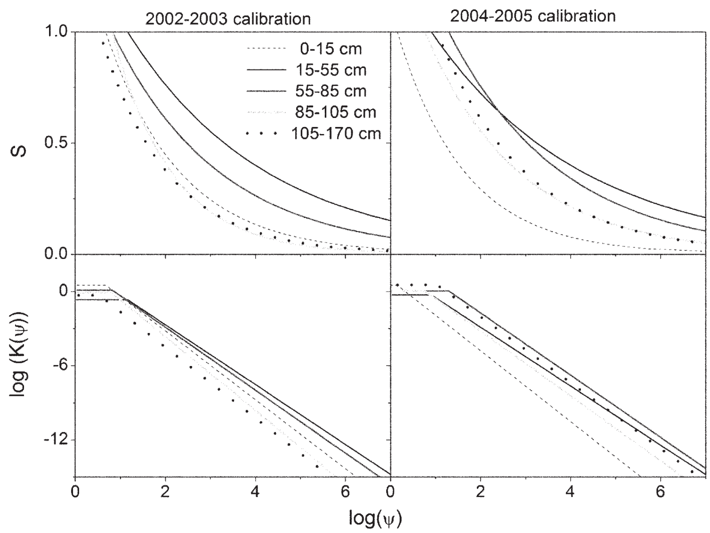

Fig. 7. The relationships of relative saturation [$S = (\theta - \theta_r)/(\theta_s - \theta_r)$, where θ, θ_r, and θ_s are measured, residual, and saturated soil water contents] and $\log_{10}$–transformed soil hydraulic conductivity [log ($K(\psi)$)], K in cm h^{-1}) versus $\log_{10}$–transformed matric suction (log(ψ), ψ in cm] for the two calibration periods (2002–2003 and 2004–2005) and each individual layer based on the parameters calibrated by Latin hypercube sampling + PEST parameter estimation program for the SWRC1K_{in} one-parameter method at Site E2.

The relationship between the calibrated values of K_{sat} and effective porosity ($\theta_s - \theta_{1/3}$) and between $\theta_{1/3}$ and θ_{15} at each individual layer across four of the methods are presented in Fig. 9. The increase in K_{sat} with increasing values of effective porosity for the SWRC1K_{es} and SWRC2K_{es} methods follows from Eq. [10]. For the other two methods with independent K_{sat} calibration, values of K_{sat} did not follow this functional relationship with $\theta_s - \theta_{1/3}$, and there was substantial scatter. From these results, we conclude that Eq. [10] overestimated K_{sat} for ($\theta_s - \theta_{1/3}$) > 0.3 (Fig. 9a). The value of K_{sat} can be calibrated first based on its relation with effective porosity or soil texture (Ahuja et al., 1984, 1989; Rawls et al., 1982) and can be further optimized manually or automatically based on a reasonable range of K_{sat} values. A strong positive relation between $\theta_{1/3}$ and θ_{15} (Fig. 9b) was found for the one-parameter method, where θ_{15} was estimated from Eq. [8]. The small deviations around the deterministic relationship between $\theta_{1/3}$ and θ_{15} for the one-parameter estimation method were caused mainly by the variations in residual water content (θ_r) sampled by LHS. Estimated θ_{15} values from the two-parameter methods were generally higher than the values calibrated from the one-parameter methods when $\theta_{1/3}$ was <0.25 m^3 m^{-3}, and the opposite results were found when $\theta_{1/3}$ was >0.25 m^3 m^{-3}. The one-parameter method also produced a few pairs of $\theta_{1/3}$ and θ_{15} substantially lower than the lower limits using the two-parameter method.

The variations in calibrated parameters between methods and data sets indicate large uncertainties in calibrating soil hydraulic parameters in RZWQM2 (Table 6). Such variations exist regardless of the parameter optimization procedures used. Higher relative mean difference (RMD) values in K_{sat} than in $\theta_{1/3}$ occurred across the different methods and data sets. In another study, obvious differences in calibrated soil hydraulic parameter values for the SWAT model were found between extrapolation and interpolation calibration–validation procedures (Sheikh and van Loon, 2007). Some reasons other than errors in the measured data were associated with the changes in soil hydraulic parameters due to tillage practices (Ahuja et al., 1984, 1998) and improper or insufficient calibration due to data limitations, even with a relatively rich temporal data set.

The six methods tested in RZWQM2 also produced different parameter values with these calibration procedures and data sets. When the measured data at all 10 depths or the selected four depths (30, 60, 90, and 120 cm) were used for Site E2, very similar values of $\theta_{1/3}$ were obtained for the six methods, indicating that the vertical resolution in measured soil water (10 vs. four depths) had little effect on $\theta_{1/3}$. Based on the mean RMD for K_{sat} across all layers, the effect of spatial (vertical) data resolution was much less than the effect of temporal data and estimation methods. Our results indicate that soil water measurements at the four depths were adequate for calibrating soil hydraulic parameters in RZWQM2 at the experimental site. As noted above, however, an additional sensor in the near-surface layer (0–15 cm) would probably have improved the simulated infiltration, runoff, and soil evaporation.

The variability in the calibrated soil hydraulic parameters in RZWQM2 among the different data sets in the case study (Table 6) was partly associated with the high sensitivity of the automatic calibration procedures (PEST) to the temporal calibration data sets. The different calibrated parameters for the six parameter estimation methods illustrates the parameter uncertainty problem of non-uniqueness as defined by Beven and Binley (1992) and as reported in other studies (Duan et al., 1992; Yapo et al., 1998; Vrugt et al., 2003b).

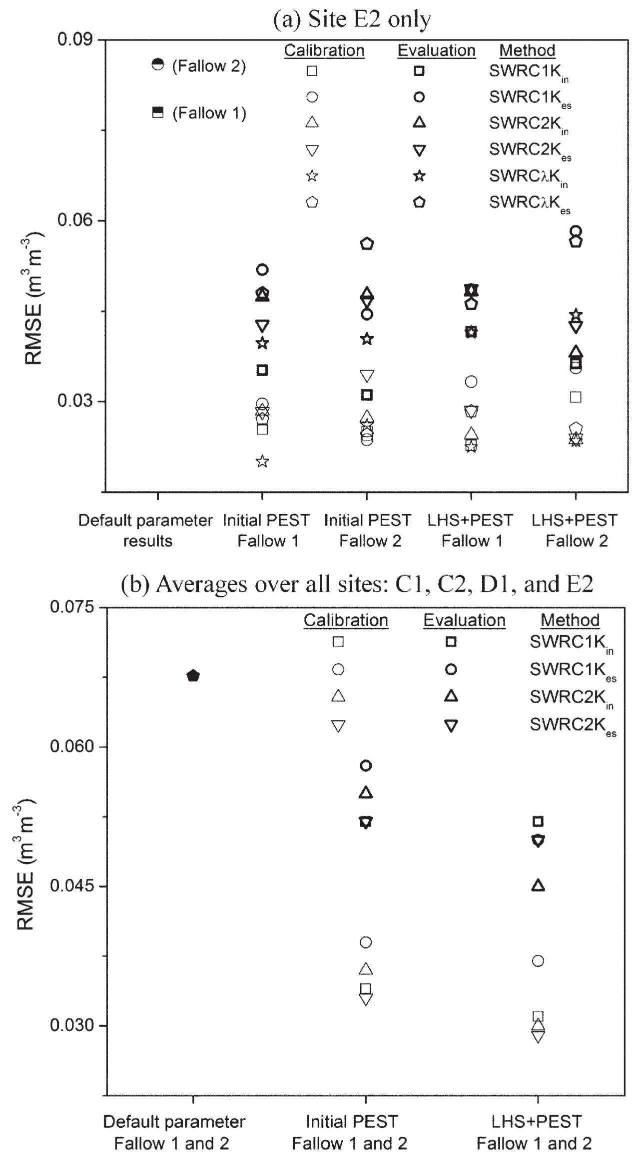

Fig. 8. Comparisons between the different calibration strategies of the PEST parameter estimation program and the combination of Latin hypercube sampling and PEST (LHS + PEST), using the RMSE based on all soil depths at the four sites across the different parameter estimation methods. The default parameter results were based on soil type in RZWQM2 (Rawls et al., 1982). Data from Fallow 1 were measured during 2006–2007 at C1 and C2, and during 2007–2008 at D1. Data from Fallow 2 were measured during 2002–2003 at C1 and C2, and during 2005–2006 at D1. Both fallow periods were used for calibration and evaluation. The SWRC1K$_{in}$ and SWRC1K$_{es}$ are one-parameter methods, SWRC2K$_{in}$ and SWRC2K$_{es}$ are two-parameter methods, and SWRCλK$_{in}$ and SWRCλK$_{es}$ are full Brooks–Corey methods.

Our results also showed that different combinations of the parameters in RZWQM2 can result in similar simulation results from the LHS analysis, where many different combinations of these parameters can result in similar model performance (RMSE and NSME values) (Fig. 4). The problem of non-uniqueness in model calibration due to acceptable solutions for single-objective automatic procedures was also reported by Madsen (2003). There is a need for prior knowledge and auxiliary data related to these model parameters before calibration. For the current study, detailed soil evaporation and K_{sat} values

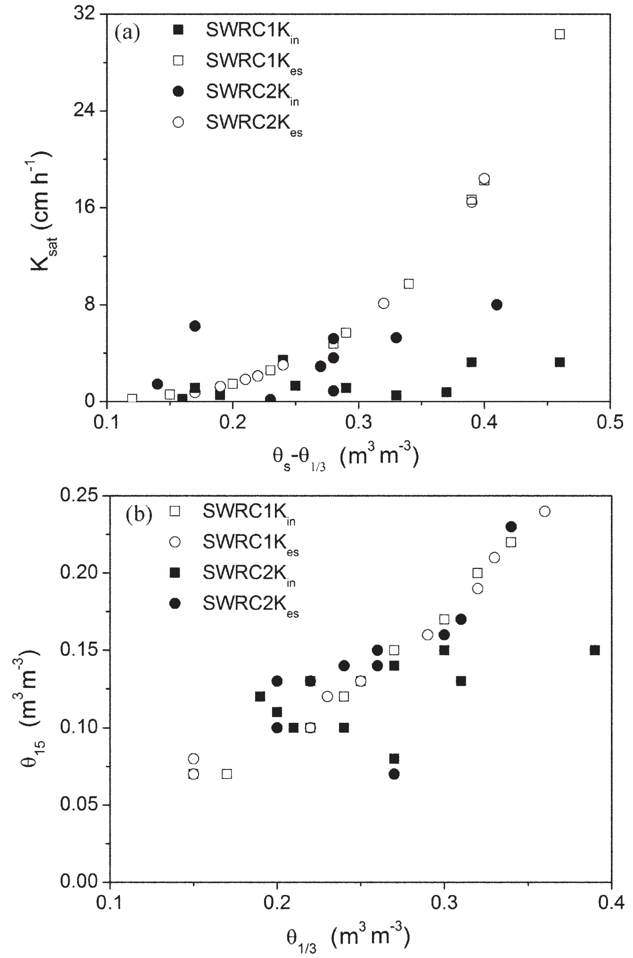

Fig. 9. Relationships between the calibrated soil hydraulic parameters of soil water content at 33 and 1500 kPa ($\theta_{1/3}$ and θ_{15}, respectively; θ_s is saturated soil water content) and saturated hydraulic conductivity (K_{sat}) for the one-parameter methods (SWRC1K$_{in}$ and SWRC1K$_{es}$) and two-parameter methods (SWRC2K$_{in}$ and SWRC2K$_{es}$) based on the results from optimization using Latin hypercube sampling combined with the PEST parameter estimation program for Site E2.

for the surface layer should be important for constraining soil hydraulic parameters in the surface layer with LHS, contributing to parameter optimization in other deeper layers, and reducing the uncertainties in parameter values in RZWQM2.

The method of measuring soil water content may be another contribution to the parameter and simulation uncertainty in this study. Measured soil water contents represented certain depth intervals, rather than averaging across full soil horizons, such as when neutron probe and time domain reflectometry methods are used. In this study, the measured soil water contents using the dielectric capacitance method represented 10-cm-thick layers. Simulated and measured soil water data were compared across the same 10-cm-thick depths, but the soil hydraulic parameters were assumed to be uniform across thicker soil horizons (see Table 3, e.g., 15–55 cm). This assumption should be further tested against observed field conditions. Increasing the number of soil horizons increases the number of parameters and their spatial interactions, which may be needed to further refine the calibrations.

Table 5. Statistical results for simulated soil water in the profiles calibrated using Latin hypercube sampling (LHS), the PEST parameter estimation program, or LHS and PEST combined at the four sites. The RMSE and Nash–Sutcliffe model efficiency (NSME) were averaged across all depths and both fallow periods for the different parameter estimation methods. The measured mean value was calculated across all the depths for the two fallow periods.

Site	Measured mean	Initial PEST program				LHS		LHS + PEST			
		Calibration		Evaluation				Calibration		Evaluation	
		RMSE	NSME	RMSE	NSME	RMSE	NSME	RMSE	NSME	RMSE	NSME
	$m^3\ m^{-3}$	$m^3\ m^{-3}$		$m^3\ m^{-3}$		$m^3\ m^{-3}$		$m^3\ m^{-3}$		$m^3\ m^{-3}$	
C1	0.186	0.039	0.461	0.075	−0.432	0.051	0.610	0.033	0.685	0.067	−0.280
C2	0.166	0.043	0.506	0.058	0.204	0.057	0.498	0.036	0.636	0.049	0.4
D1	0.176	0.031	−0.013	0.039	−0.615	0.035	0.550	0.030	0.105	0.038	−0.325
E2	0.224	0.028	0.860	0.045	0.633	0.043	0.679	0.029	0.852	0.044	0.657
Mean	0.188	0.035		0.054		0.047		0.032		0.049	

CONCLUSIONS

Six methods within RZWQM2 for estimating the BC soil hydraulic parameters were evaluated using two external optimization procedures (LHS and PEST) and their combination (LHS + PEST). Based on our results, the one-parameter method is recommended for the LHS procedure using a limited number of samples (6000). The two-parameter method can be used to further improve the calibrations, but this requires careful setting of the parameter ranges for the automatic calibration procedures as implemented here. The SWRC2K$_{in}$ method outperformed the other five internal parameter estimation methods only when used with the LHS + PEST approach. Otherwise, the one-parameter method was more efficient when using PEST or LHS alone. This is also why the one-parameter methods have been developed for manual calibration.

The combination of LHS + PEST avoided anomalous soil hydraulic parameters and soil evaporation predictions. The LHS results reduced the parameter search space and stabilized simulation results between calibration and evaluation periods compared with the initial PEST optimizations. Recent advances in other optimization procedures discussed here may be tested in future investigations using these data and periods with crop growth.

Cross-validation during different time periods identified some large deviations between simulated and measured water contents, primarily related to the timing of propagation of seasonal wetting fronts with depth. The variability of calibrated soil parameters between calibration periods implied parameter uncertainty or non-uniqueness, indicating possible structural model errors related, at least in part, to the delineation of soil horizons. Thus, more site-specific soil data and characterization of soil layers may help reduce parameter uncertainty and improve spatial and temporal aspects of simulated soil water dynamics.

The very similar calibrated parameter values based on 10 sensor depths vs. four depths indicate that soil water measurements at the four depths (e.g., 30-cm intervals) in most probes at the experimental field were adequate for calibrating soil hydraulic parameters in RZWQM2. More shallow measurements (<30 cm), however, should help with calibration of the surface soil layers that control most of the infiltration and evaporation

Table 6. Averaged relative mean difference (RMD) for the calibrated soil hydraulic parameters of soil water at 33 kPa ($q_{1/3}$) and saturated hydraulic conductivity (K_{sat}) for the different fallow periods, parameter estimation methods (SWRC1K$_{in}$, SWRC1K$_{es}$, SWRC2K$_{in}$, and SWRC2K$_{es}$), and data sets (10 or four depths) at E2 site. The ranges of RMD among the six methods are given in parentheses.

Soil depth	RMD†					
	Temporal, Fallows 1 or 2‡		Spatial, 10 or 4 depths§		Parameter estimation method¶	
	$\theta_{1/3}$	K_{sat}	$\theta_{1/3}$	K_{sat}	$\theta_{1/3}$	K_{sat}
cm	%					
0–15	29 (10–38)	28 (0–58)	0	7	18 (0–28)	105 (79–161)
15–55	12 (5–26)	108 (50–158)	1	18	9 (0–18)	97 (32–152)
55–85	15 (8–26)	94 (16–150)	0	19	14 (3–27)	65 (23–115)
85–105	23 (5–38)	52 (0–118)	0	8	11 (0–20)	78 (31–133)
105–170	33 (12–43)	87 (35–149)	3	11	9 (1–17)	32 (8–91)
Mean	22	74	1	13	12	76

†

$$RMD=\frac{2\sum_{i=1}^{L}\sum_{j=1}^{M}\left[\frac{\left|X_{ij}-Y_{ij}\right|}{\left(X_{ij}+Y_{ij}\right)}\right]}{L\times M\times N}\times 100\%$$

where i is fallow period, j is parameter method, X_{ij} and Y_{ij} are the calibrated parameter values from the different fallow periods (temporal), different measured data depths (spatial), or different parameter methods, and L = 2, M = 4, and N = 1 .

‡ RMD was calculated for the two fallow periods, Fallow 1 (2002–2003) and Fallow 2 (2004–2005), across the four parameter estimation methods.

§ RMD was calculated when the data for 10 or four depths were used for the four parameter estimation methods.

¶ RMD was calculated for the four parameter estimation methods.

fluxes. Also, soil parameter interactions across horizons affect the space–time distribution of soil water.

This case study in a semiarid climate illustrates how soil hydraulic parameters can be optimized using different automated calibration procedures evaluated by cross-validation with time. In future work, the different parameter estimation methods in RZWQM2 should be compared further under a broader range of site conditions, such as more humid climates and clayey soils, using advanced optimization procedures.

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REFERENCES

Abbaspour, K.C., C.A. Johnson, and M.Th. van Genuchten. 2004. Estimating uncertain flow, and transport parameters using a sequential uncertainty fitting procedure. Vadose Zone J. 3:1340–1352.

Ahuja, L.R., D.K. Cassel, R.R. Bruce, and B.B. Barnes. 1989. Evaluation of spatial distribution of hydraulic conductivity using effective porosity data. Soil Sci. 148:404–411.

Ahuja, L.R., F. Fiedler, G.H. Dunn, J.G. Benjamin, and A. Garrison. 1998. Changes in soil water retention curves due to tillage and natural reconsolidation. Soil Sci. Soc. Am. J. 62:1228–1233.

Ahuja, L.R., and L. Ma. 2002. Parameterization of agricultural system models: Current approaches and future needs. p. 273–316. *In* L.R. Ahuja et al. (ed.) Agricultural System models in field research and technology transfer. Lewis Publ., London.

Ahuja, L.R., L.W. Ma, and D.J. Timlin. 2006. Trans-disciplinary soil physics research critical to synthesis and modeling of agricultural systems. Soil Sci. Soc. Am. J. 70:311–326.

Ahuja, L.R., J.W. Naney, R.E. Green, and D.R. Nielsen. 1984. Macroporosity to characterize spatial variability of hydraulic conductivity and effects of land management. Soil Sci. Soc. Am. J. 48:699–702.

Ahuja, L.R., J.W. Naney, and R.D. Williams. 1985. Estimating soil-water characteristics from simpler properties or limited data. Soil Sci. Soc. Am. J. 49:1100–1105.

Ahuja, L.R., W.J. Rawls, and D. Nielson. 1999. Determining soil hydraulic properties and their field variability from simpler measurements. Agron. J. 38:1207–1234.

Ahuja, L.R., K.W. Rojas, J.D. Hanson, M.J. Shaffer, and L. Ma (ed.). 2000. The Root Zone Water Quality Model. Water Resour. Publ., Highlands Ranch, CO.

Ahuja, L.R., and R.D. Williams. 1991. Scaling water characteristic and hydraulic conductivity based on Gregson–Hector–McGowan approach. Soil Sci. Soc. Am. J. 55:308–319.

Beven, K., and A. Binley. 1992. The future of distributed models: Model calibration and uncertainty prediction. Hydrol. Processes 6:279–298.

Børgesen, C.D., B.V. Iversen, O.H. Jacobsen, and M.G. Schaap. 2008. Pedotransfer functions estimating soil hydraulic properties using different soil parameters. Hydrol. Processes 22:1630–1639.

Bouma, J. 1989. Using soil survey data for quantitative land evaluation. Adv. Soil Sci. 9:177–213.

Bouma, J., and H.A.J. van Lanen. 1987. Transfer functions and threshold values: From soil characteristics to land qualities. p. 106–110. *In* K.J. Beek et al. (ed.) Quantified land evaluation. ITC Publ. 6. Int. Inst. for Aerospace Surv. and Earth Sci., Enschede, the Netherlands.

Brooks, R., and A. Corey. 1964. Hydraulic properties of porous media. Hydrol. Pap. 3. Colorado State Univ., Fort Collins.

Burt, C.M., A.J. Mutziger, R.G. Allen, and T.A. Howell. 2005. Evaporation research: Review and interpretation. J. Irrig. Drain. Eng. 131:37–59.

Chirico, G.B., H. Medina, and N. Romano. 2007. Uncertainty in predicting soil hydraulic properties at the hillslope scale with indirect methods. J. Hydrol. 334:405–422.

Christiaens, K., and J. Feyen. 2002. Constraining soil hydraulic parameter and output uncertainty of the distributed hydrological MIKE SHE model using the GLUE framework. Hydrol. Processes 16:373–391.

Doherty, J. 2004. PEST model: Independent parameter estimation. User manual. 5th ed. Watermark Numerical Comput., Corinda, QLD, Australia.

Duan, Q.Y., S. Sorooshian, and V. Gupta. 1992. Effective and efficient global optimization for conceptual rainfall–runoff models. Water Resour. Res. 28:1015–1031.

Fang, Q., L. Ma, Q. Yu, L.R. Ahuja, R.W. Malone, and G. Hoogenboom. 2010. Irrigation strategies to improve the water use efficiency of wheat–maize double cropping systems in North China Plain. Agric. Water Manage. 97:1165–1174.

Fang, Q., L. Ma, Q. Yu, R.W. Malone, S.A. Saseendran, and L.R. Ahuja. 2008. Modeling nitrogen and water management effects in a wheat–maize double-cropping system. J. Environ. Qual. 37:2232–2242.

Green, T.R., L.R. Ahuja, and J.G. Benjamin. 2003. Advances and challenges in predicting agricultural management effects on soil hydraulic properties. Geoderma 116:3–27.

Green, T.R., J.E. Constantz, and D.L. Freyberg. 1996. Upscaled soil-water retention using van Genuchten's function. J. Hydrol. Eng. 1:123–130.

Green, T.R., G.H. Dunn, R.H. Erskine, J.D. Salas, and L.R. Ahuja. 2009. Fractal analyses of steady infiltration and terrain on an undulating agricultural field. Vadose Zone J. 8:310–320.

Gupta, H.V., S. Sorooshian, T.S. Hogue, and D.P. Boyle. 2003. Advances in automatic calibration of watershed models. p. 9–28. *In* Q.Y. Duan et al. (ed.) Calibration of watershed models. Am. Geophys. Union, Washington, DC.

Hopmans, J.W., J. Šimůnek, N. Romano, and W. Durner. 2002. Simultaneous determination of water transmission and retention properties: Inverse methods. p. 963–1008. *In* J.H. Dane and G.C. Topp (ed.) Methods of soil analysis. Part 4. Physical methods. SSSA Book Ser. 5. SSSA, Madison, WI.

Hu, C., S.A. Saseendran, T.R. Green, L. Ma, X. Li, and L.R. Ahuja. 2006. Evaluating nitrogen and water management in a double-cropping system using RZWQM. Vadose Zone J. 5:493–505.

Huisman, J.A., J. Rings, J.A. Vrugt, J. Sorg, and H. Vereecken. 2010. Hydraulic properties of a model dike from coupled Bayesian and multi-criteria hydrogeophysical inversion. J. Hydrol. 380:62–73.

Hupet, F., S. Lambot, R.A. Feddes, J.C. van Dam, and M. Vanclooster. 2003. Estimation of root water uptake parameters by inverse modeling with soil water content data. Water Resour. Res. 39(11):1312, doi:10.1029/2003WR002046.

Hupet, F., J.C. van Dam, and M. Vanclooster. 2004. Impact of within-field variability in soil hydraulic properties on transpiration fluxes and crop yields: A numerical study. Vadose Zone J. 3:1367–1379.

Iskra, I., and R. Droste. 2007. Application of non-linear automatic optimization techniques for calibration of HSPF. Water Environ. Res. 79:647–659.

Jhorar, R.K., J.C. van Dam, W.G.M. Bastiaanssen, and R.A. Feddes. 2004. Calibration of effective soil hydraulic parameters of heterogeneous soil profiles. J. Hydrol. 285:233–247.

Kuzmin, V., D.J. Seo, and V. Koren. 2008. Fast and efficient optimization of hydrologic model parameters using a priori estimates and stepwise line search. J. Hydrol. 353:109–128.

Ma, L., L.R. Ahuja, and R.W. Malone. 2007. Systems modeling for soil and water research and management: Current status and needs for the 21st century. Trans. Am. Soc. Agric. Biol. Eng. 50:1705–1713.

Ma, L., G. Hoogenboom, S.A. Saseendran, P.N. Bartling, L.R. Ahuja, and T.R. Green. 2009. Effects of estimating soil hydraulic properties and root growth factor on soil water balance and crop production. Agron. J. 101:572–583.

Madsen, H. 2003. Parameter estimation in distributed hydrological catchment modelling using automatic calibration with multiple objectives. Adv. Water Resour. 26:205–216.

Madsen, H., G. Wilson, and H.C. Ammentrop. 2002. Comparison of different automated strategies for calibration of rainfall–runoff models. J. Hydrol. 261:48–59.

Maneta, M.P., S. Schnabel, W.W. Wallender, S. Panday, and V. Jetten. 2008. Calibration of an evapotranspiration model to simulate soil water dynamics in a semiarid rangeland. Hydrol. Processes 22:4655–4669.

Marshall, L., D. Nott, and A. Sharma. 2004. A comparative study of Markov chain Monte Carlo methods for conceptual rainfall–runoff modeling. Water Resour. Res. 40:W02501, doi:10.1029/2003WR002378.

McKay, M.D., W.J. Conover, and R.J. Beckman. 1979. A comparison of three

methods for selecting values of input variables in the analysis of output from a computer code. Technometrics 21:239–245.
Meadows, D.G., M.H. Young, and E.V. McDonald. 2005. A laboratory method for determining the unsaturated hydraulic properties of soil peds. Soil Sci. Soc. Am. J. 69:807–815.
Mertens, J., H. Madsen, M. Kristensen, D. Jacques, and J. Feyen. 2005. Sensitivity of soil parameters in unsaturated zone modelling and the relation between effective, laboratory and in situ estimates. Hydrol. Processes 19:1611–1633.
Nash, J.E., and J.V. Sutcliffe. 1970. River flow forecasting through conceptual models: I-A. Discussion of principles. J. Hydrol. 10:282–290.
Nolan, B.T., L.J. Puckett, L. Ma, C.T. Green, E.R. Bayless, and R.W. Malone. 2010. Predicting unsaturated zone nitrogen mass balances in agricultural settings of the United States. J. Environ. Qual. 39:1051–1065.
Oliver, Y.M., and K.R.J. Smettem. 2005. Predicting water balance in a sandy soil: Model sensitivity to the variability of measured saturated and near saturated hydraulic properties. Aust. J. Soil Res. 43:87–96.
Rawls, W.J., D.L. Brakensiek, and K.E. Saxton. 1982. Estimation of soil-water properties. Trans. Am. Soc. Agric. Eng. 25:1316–1320, 1328.
Rawls, W.J., T.J. Gish, and D.L. Brakensiek. 1991. Estimation of soil water retention from soil properties: A review. Adv. Soil Sci. 16:213–235.
Romano, N., and A. Santini. 1999. Determining soil hydraulic functions from evaporation experiments by a parameter estimation approach: Experimental verifications and numerical studies. Water Resour. Res. 35:3343–3359.
Schwank, M., T.R. Green, C. Mätzler, H. Benedickter, and H. Flühler. 2006. Laboratory characterization of a commercial capacitance sensor for estimating permittivity and inferring soil water content. Vadose Zone J. 5:1048–1064.
Shan, S., and G.G. Wang. 2009. Survey of modeling and optimization strategies to solve high-dimensional design problems with computationally-expensive black-box functions. Struct. Multidiscip. Optim. 41:219–241.
Sheikh, V., and E.E. van Loon. 2007. Comparing performance and parameterization of a one-dimensional unsaturated zone model across scales. Vadose Zone J. 6:638–650.
Simmons, C.S., D.R. Nielsen, and J.W. Biggar. 1979. Scaling of field-measured soil-water flow and solute properties: 2. Hydraulic conductivity and flux. Hilgardia 47:77–102.
Skahill, B.E., J.S. Baggett, S. Frankenstein, and C.W. Downer. 2009. More efficient PEST compatible model independent model calibration. Environ. Modell. Softw. 24:517–529.
Skahill, B.E., and J. Doherty. 2006. Efficient accommodation of local minima in watershed model calibration. J. Hydrol. 329:122–139.
Si, B.C., and R.G. Kachanoski. 2000. Estimating soil hydraulic properties during constant flux infiltration: Inverse procedures. Soil Sci. Soc. Am. J. 64:439–449.
Sorooshian, S., and V.K. Gupta. 1995. Model calibration. p. 23–68. *In* V.P. Singh (ed.) Computer models of watershed hydrology. Water Resour. Publ., Highlands Ranch, CO.
Strudley, M.W., T.R. Green, and J.C. Ascough II. 2008. Tillage effects on soil hydraulic properties in space and time: State of the science. Soil Tillage Res. 99:4–48.
Sumner, N.R., P.M. Fleming, and B.C. Bates. 1997. Calibration of a modified SFB model for twenty-five Australian catchments using simulated annealing. J. Hydrol. 197:166–188.
Twarakavi, N.K.C., H. Saito, J. Šimůnek, and M.Th. van Genuchten. 2008. A new approach to estimate soil hydraulic parameters using only soil water retention data. Soil Sci. Soc. Am. J. 72:471–479.
van Dam, J.C., J.N.M. Stricker, and P. Droogers. 1994. Inverse method for determining soil hydraulic functions from multi-step outflow experiments. Soil Sci. Soc. Am. J. 58:647–652.
van Genuchten, M.Th., and F. Leij. 1992. On estimating the hydraulic properties of unsaturated soils. p. 1–14. *In* M.Th. van Genuchten et al. (ed.) Proc. Int. Worksh. on Indirect Methods of Estimating the Hydraulic Properties of Unsaturated Soils, Riverside, CA. 11–13 Oct. 1989. U.S. Salinity Lab., Riverside, CA.
van Griensven, A., T. Meixner, S. Grunwald, T. Bishop, A. Diluzio, and R. Srinivasan. 2006. A global sensitivity analysis tool for the parameters of multi-variable catchment models. J. Hydrol. 324:10–23.
Vrugt, J.A., W. Bouten, H.V. Gupta, and J.W. Hopmans. 2003a. Toward improved identifiability of soil hydraulic parameters: On selection of a suitable parametric model. Vadose Zone J. 2:98–113.
Vrugt, J.A., H.V. Gupta, W. Bouten, and S. Sorooshian. 2003b. A Shuffled Complex Evolution Metropolis algorithm for optimization and uncertainty assessment of hydrologic model parameters. Water Resour. Res. 39(8):1201, doi:10.1029/2002WR001642.
Vrugt, J.A., and B.A. Robinson. 2007. Improved evolutionary optimization from genetically adaptive multimethod search. Proc. Natl. Acad. Sci. 104:708–711.
Vrugt, J.A., P.H. Stauffer, T. Wöhling, B.A. Robinson, and V.V. Vesselinov. 2008. Inverse modeling of subsurface flow and transport properties: A review with new developments. Vadose Zone J. 7:843–864.
Vrugt, J.A., C.J.F. Ter Braak, C.G.H. Diks, B.A. Robinson, J.M. Hyman, and D. Higdon. 2009. Accelerating Markov chain Monte Carlo simulation by differential evolution with self-adaptive randomized subspace sampling. Int. J. Nonlin. Sci. Numer. Simul. 10:273–290.
Wagener, T., N. McIntyre, M.J. Lees, H.S. Wheater, and H.V. Gupta. 2003. Towards reduced uncertainty in conceptual rainfall–runoff modelling: Dynamic identifiability analysis. Hydrol. Processes 17:455–476.
Wang, Q.J. 1991. The genetic algorithm and its application to calibrating conceptual rainfall–runoff models. Water Resour. Res. 27:2467–2471.
Warrick, A.W., G.J. Mullen, and D.R. Nielsen. 1977. Scaling field-measured soil hydraulic properties using a similar media concept. Water Resour. Res. 13:355–362.
Williams, R.D., and L.R. Ahuja. 1992. Evaluation of similar-media scaling and a one-parameter model for estimating the soil-water characteristic. J. Soil Sci. 43:237–248.
Williams, R.D., and L.R. Ahuja. 2003. Scaling and estimating the soil water characteristic using a one-parameter model. p. 35–48. *In* Y. Pachepsky et al. (ed.) Scaling methods in soil physics. CRC Press, Boca Raton, FL.
Wöhling, Th., J.A. Vrugt, and G.F. Barkle. 2008. Comparison of three multiobjective optimization algorithms for inverse modeling of vadose zone hydraulic parameters. Soil Sci. Soc. Am. J. 72:305–319.
Wösten, J.H.M., Y.A. Pachepsky, and W.J. Rawls. 2001. Pedotransfer functions: Bridging the gap between available basic soil data and missing soil hydraulic characteristics. J. Hydrol. 251:123–150.
Yapo, P.O., H.V. Gupta, and S. Sorooshian. 1998. Multi-objective global optimization for hydrologic models. J. Hydrol. 203:83–97.
Yu, Q., S.A. Saseendran, L. Ma, G.N. Flerchinger, T.R. Green, and L.R. Ahuja. 2006. Modeling a wheat–maize double cropping system in China using two plant growth modules in RZWQM. Agric. Syst. 89:457–477.