Optimizing Soil Hydraulic Parameters in RZWQM2 under Fallow Conditions

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 (Borgesen 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 soil hydraulic parameters.

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 six 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–Marquardt–Levenberg; LHS, Latin hypercube sampling; NSME, Nash–Sutcliffe model efficiency; RZWQM2, Root Zone Water Quality Model; SWRC, soil water retention curve.
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 multi-method 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 ψ > 0 for negative soil water pressures) are
where \( \theta_s \) and \( \theta_r \) are saturated and residual soil water contents, respectively, \( \psi \), is the air-entry water suction (negative “bubbling pressure head”), and \( \lambda \) is the absolute value of the slope of the \( \log(\theta) - \log(\psi) \) 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

\[
K(\psi) = K_{sat} \left( \frac{\psi}{\psi_b} \right)^{-\lambda} \quad \text{for } \psi < \psi_b
\]

\[
K(\psi) = K_{sat} \left( \frac{\psi}{\psi_b} \right)^{-1/3} \quad \text{for } \psi \geq \psi_b
\]

where \( K_{sat} \) is the saturated hydraulic conductivity. Therefore, the “full” set of BC parameters for both water retention and conductivity include \( K_{sat}, \theta_s, \theta_r, \psi_b, \) and \( \lambda \).

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 this 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 \( \theta \) and \( \psi \) can be written as (Ahuja and Williams, 1991)

\[
\ln(\psi) = a + b \ln(\theta_1/\theta_r)
\]

where \( a = p + q \beta \) and \( b = -1/\lambda \). Williams and Ahuja (1992) found that

\[
a = p + q \beta
\]

where \( p = -0.52 \) and \( q = 0.67 \) for all soil texture classes when \( \psi \) is in kilopascals. The value of \( \lambda \) is calculated from \( \theta_s \) and \( \theta_s^{1/3} \) (soil water content at 33 kPa or 1/3 bar), and then \( \psi_b \) is obtained from \( a \) and \( \lambda \), 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 \( \theta_s \) (assuming \( \theta_r \) is measured and \( \theta_r = 0 \) or a known value), it is called the one-parameter method. In this study, \( \theta_1 \) and \( \theta_r \) are added unknowns, but with smaller bounds.

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

\[
\ln(333) = a + b \ln(\theta_s^{1/3} - \theta_r^{1/3})
\]

\[
\ln(15,000) = a + b \ln(\theta_s^{1/3} - \theta_r^{1/3})
\]

From these two equations, \( \lambda \) is

\[
\lambda = \frac{\ln\left(\frac{\theta_s^{1/3} - \theta_r^{1/3}}{\theta_s^{1/3} - \theta_r^{1/3}}\right)}{\ln(15,000/333)}
\]

Because both \( \theta_s^{1/3} \) and \( \theta_r^{1/3} \) are needed for estimating the soil water retention curve, it is called the two-parameter method.

The third method was based on the parameters \( \lambda, \psi_b, \theta_s \), and \( \theta_r \) 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., \( \theta_s^{1/3} \) and \( \theta_r^{1/3} \)) 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:

\[
K_{sat} = 509.4 (\theta_s^{1/3} - \theta_r^{1/3})^{2.63}
\]

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 SWRCCK\(_{in}\) and SWRCCK\(_{es}\) 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 al., 2007a), were also employed.

### 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.

<table>
<thead>
<tr>
<th>Method</th>
<th>( K_{sat} ) estimated from Eq. [10]</th>
<th>Calibration parameters†</th>
<th>Optimization procedures</th>
</tr>
</thead>
<tbody>
<tr>
<td>One-parameter method</td>
<td>SWRC1K(_{in})</td>
<td>( \theta_s, \theta_s^{1/3}, K_{sat} )</td>
<td>PEST, LHS, LHS + PEST</td>
</tr>
<tr>
<td>Two-parameter method</td>
<td>SWRC2K(_{in})</td>
<td>( \theta_s, \theta_s^{1/3}, \theta_r^{1/3}, K_{sat} )</td>
<td>PEST, LHS + PEST</td>
</tr>
<tr>
<td>Full Brooks–Corey method</td>
<td>SWRCCK(_{in})</td>
<td>( \theta_s, \lambda, \psi_b, K_{sat} )</td>
<td>PEST, LHS, LHS + PEST</td>
</tr>
</tbody>
</table>

† \( \theta_s \), saturated soil water content (m\(^3\) m\(^{-3}\)); \( \theta_s^{1/3} \) and \( \theta_r^{1/3} \), soil water contents at 33 and 1500 kPa (m\(^3\) m\(^{-3}\)); \( K_{sat} \), saturated hydraulic conductivity (cm h\(^{-1}\)); \( \lambda \), pore-size distribution index; \( \psi_b \), 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, $\theta_s$, $\theta_r$, $\theta_{1/3}$, $\lambda$, $\psi_b$ 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:

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

where $F$ is a set of fitting parameters, $O(t_i)$ is the observation at the $i$th time, $P(F, t_i)$ is the model prediction at the $i$th time, and $w_i$ is the weighting factor for the $i$th 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
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 (Fallow 1 (2002–2003 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\textsubscript{in} and SWRC2K\textsubscript{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:

\[
\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (O_i - P_i)^2} \tag{12}
\]

\[
\text{NSME} = 1.0 - \frac{\sum_{i=1}^{n} (O_i - P_i)^2}{\sum_{i=1}^{n} (O_i - O_{avg})^2} \tag{13}
\]

where \(P_i\) is the \(i\)th predicted value, \(O_i\) is the \(i\)th 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 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.

### 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.

<table>
<thead>
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<tr>
<td>Min.</td>
<td>Max.</td>
<td>Mean</td>
</tr>
<tr>
<td>30</td>
<td>0.15</td>
<td>0.40</td>
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<tr>
<td>40</td>
<td>0.18</td>
<td>0.40</td>
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<tr>
<td>50</td>
<td>0.18</td>
<td>0.39</td>
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<td>60</td>
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<tr>
<td>70</td>
<td>0.14</td>
<td>0.34</td>
</tr>
<tr>
<td>80</td>
<td>0.15</td>
<td>0.33</td>
</tr>
<tr>
<td>90</td>
<td>0.12</td>
<td>0.24</td>
</tr>
<tr>
<td>100</td>
<td>0.10</td>
<td>0.15</td>
</tr>
<tr>
<td>120</td>
<td>0.12</td>
<td>0.16</td>
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<tr>
<td>150</td>
<td>0.13</td>
<td>0.17</td>
</tr>
<tr>
<td>170</td>
<td>0.13</td>
<td>0.17</td>
</tr>
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</table>

\(\Delta\text{SWC}^\dagger\) is the difference in soil water content at each depth between the beginning and end of the period.

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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 SWRC1KI and SWRC1Ke methods generally produced better simulation results than the other methods. Abnormal soil evaporation occurred for the two-parameter methods (SWRC2KI and SWRC2Ke), however, with simulated annual soil evaporation values of <6 cm (only about 18% of rainfall) associated with unreasonable combinations of the soil hydraulic parameters \( \theta_{1/3} \), \( \theta_{15} \), 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 (\( \theta_{s} \)) 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).

**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 \( \theta_{s} \), \( \theta_{h} \), \( \theta_{1/3} \), 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 \( \theta_{s} \) 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 \( \theta_{s} \) 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 (SWRC2KI and SWRC2Ke),

![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 SWRC1KI and SWRC1Ke are one-parameter methods, SWRC2KI and SWRC2Ke are two-parameter methods, and SWRC1Kes and SWRC2Kes are full Brooks–Corey methods.](image-url)
unreasonable combinations of $\theta_{1/3}$ and $\theta_{15}$ occurred when sampling the two parameters using the LHS method. Instead, we sampled the parameters $\theta$, $K_{sat}$, $\lambda$, and $\psi_b$ for the full BC method (SWRC\(\lambda\)K\(s\)_in and SWRC\(\lambda\)K\(s\)_es) based on soil type for each layer in RZWQM2, then calculated $\theta_{1/3}$ and $\theta_{15}$ 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 $\lambda$ from $\theta_{1/3}$ were mainly due to the variations in $\theta$ and $\lambda$. The relationship between $\theta_{1/3}$ and $\theta_{15}$ for SWRC\(\lambda\)K\(s\)_es showed a linear correlation, with a larger deviation than for the SWRC\(\lambda\)K\(s\)_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 SWRC\(\lambda\)K\(s\)_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 SWRC\(\lambda\)K\(s\)_in and SWRC\(\lambda\)K\(s\)_es (Fig. 4g and 4h) and the optimal range of the pore size distribution parameter $\lambda$ for SWRC\(\lambda\)K\(in\) (Fig. 4f). No obvious relationship between model performance and $\psi_b$ was found (Fig. 4c), however. No obvious relationship between model performance and $K_{sat}$ was found for the SWRC\(\lambda\)K\(in\) method (Fig. 4i), indicating less parameter correlation than assumed using SWRC\(\lambda\)K\(es\) (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 $\theta_{15}$ were highly correlated with $\lambda$, 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 SWRC\(\lambda\)K\(in\), but similar to SWRC\(\lambda\)K\(es\) (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
Table 3. Calibrated soil hydraulic parameters of soil water content at 33 kPa and 1500 kPa ($\theta_{1/3}$ and $\theta_{15}$) 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.

<table>
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<tr>
<th>Method and data set</th>
<th>Depth</th>
<th>SWRC1K&lt;sub&gt;in&lt;/sub&gt;</th>
<th>SWRC1K&lt;sub&gt;es&lt;/sub&gt;</th>
<th>SWRC2K&lt;sub&gt;in&lt;/sub&gt;</th>
<th>SWRC2K&lt;sub&gt;es&lt;/sub&gt;</th>
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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 SWRCXK$_{in}$ and SWRCXK$_{es}$, but showed similar trends with soil depth (Table 3). Across the six methods, the selected parameter values of $\theta_{1/3}$ and $\theta_{15}$ 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 SWRCXK$_{es}$ methods than for the SWRC1K$_{in}$ and SWRCXK$_{in}$ 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
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 SWRC1Kes and SWRC1Kes 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 \( \theta_{1/3}, \theta_{15} \) and \( K_{sat} \) for SWRC1Kin were generally lower than for the other methods; using 2004–2005 fallow data for calibration, these parameters for SWRC2Kin were relatively lower than the other methods except for in the surface layer. The resulting water retention characteristics and hydraulic conductivity curves for SWRC1Kin (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 SWRC1Kin and SWRC2Kin 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).
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.
optimization. For Sites C1 and C2, the relative RMSE (RMSE/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 SWRC1Kin 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 SWRC2Kin 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.

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 SWRC1Kin and SWRC1Kes are one-parameter methods, SWRC2Kin and SWRC2Kes are two-parameter methods, and SWRCxKin and SWRCxKes are full Brooks–Corey methods.
The parameters calibrated by the LHS + PEST procedure for the six methods are presented in Table 3. Similar trends in $\theta_{1/3}$, $\theta_{15}$, and $K_{\text{sat}}$ occurred with soil depth among the parameter estimation methods, but large differences in $K_{\text{sat}}$ were found between the two different methods of estimating $K_{\text{sat}}$ (denoted $K_{\text{in}}$ and $K_{\text{es}}$). Across the six methods, no significant differences in the values of $\theta_s$, $\theta_{1/3}$, and $\theta_{15}$ 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 $\theta_{15}$ 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.

The relationship between the calibrated values of $K_{\text{sat}}$ and effective porosity ($\theta_{1/3}$) and between $\theta_{1/3}$ and $\theta_{15}$ at each individual layer across four of the methods are presented in Fig. 9. The increase in $K_{\text{sat}}$ 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 $K_{\text{sat}}$ calibration, values of $K_{\text{sat}}$ 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 $K_{\text{sat}}$ for $\theta_s - \theta_{1/3} > 0.3$ (Fig. 9a). The value of $K_{\text{sat}}$ 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 $K_{\text{sat}}$ values. A strong positive relation between $\theta_{1/3}$ and $\theta_{15}$ (Fig. 9b) was found for the one-parameter method, where $\theta_{15}$ was estimated from Eq. [8]. The small deviations around the deterministic relationship between $\theta_{1/3}$ and $\theta_{15}$ for the one-parameter estimation method were caused mainly by the variations in residual water content ($\theta_s$) sampled by LHS. Estimated $\theta_{15}$ 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 $\theta_{15}$ 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 $K_{\text{sat}}$ 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 $K_{\text{sat}}$ 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 illustrate 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).
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 $K_{\text{sat}}$ values 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.
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>
<thead>
<tr>
<th>Soil depth (cm)</th>
<th>0–15</th>
<th>15–55</th>
<th>55–85</th>
<th>85–105</th>
<th>105–170</th>
<th>Mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>θ1/3 (m³ m⁻³)</td>
<td>29 (10–38)</td>
<td>12 (5–26)</td>
<td>15 (8–26)</td>
<td>23 (5–38)</td>
<td>33 (12–43)</td>
<td>22</td>
</tr>
<tr>
<td>Ksat (m³ m⁻³)</td>
<td>28 (0–58)</td>
<td>108 (50–158)</td>
<td>94 (16–150)</td>
<td>52 (0–118)</td>
<td>87 (35–149)</td>
<td>74</td>
</tr>
</tbody>
</table>

where \( i \) is fallow period, \( j \) is parameter method, \( X_\alpha \) and \( Y_\alpha \) 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.
fl uxes. 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


