Soil Hydraulic Modeling Outcomes with Four Parameterization Methods: Comparing Soil Description and Inverse Estimation Approaches

Scott L. Graham,* M.S. Srinivasan, Nathalie Faulkner, and Sam Carrick

Different methods for parameterizing soil hydraulic models can lead to substantially varied predictions of soil–plant–atmosphere water fluxes. This study investigated, for a heterogeneous stony soil, four methods of soil hydraulic parameterization: (i) use of a pedotransfer function with a four-layer soil profile based on detailed soil physical and textural description; (ii) use of a pedotransfer function with a single-layer soil description; (iii) inverse estimation from soil moisture data; and (iv) inverse estimation from lysimeter drainage. Soil drainage, volumetric water content, and evapotranspiration were each modeled using HYDRUS-1D for an irrigated pasture in New Zealand during the time period 1 July 2011 to 15 Mar. 2014. The first 15 mo were used for model spin-up and inverse parameter estimation, while the remainder of the study period was used as a validation period, during which model results were compared against field data. Predictions from each model parameterization were compared with field-measured fluxes from lysimeter, soil moisture sensors, and eddy covariance to determine the approach most appropriate for our site and application. The parameters estimated inversely from field data improved the modeling of soil drainage, leading to total drainage within 5 to 7% of the measured volume and prediction of 35 to 80% more drainage peaks than parameterizations based on detailed soil physical description. While all methods underpredicted evapotranspiration by 18 to 30% compared with eddy covariance, improvement in drainage estimates with inverse estimation from field data led to decreased capability for modeling evapotranspiration. We suggest this approach for application in other settings to select the most appropriate parameterization approach for a given soil hydraulic model application.

Abbreviations: ET, evapotranspiration; NSE, Nash–Sutcliffe efficiency.

It is widely accepted that each of the available methods for estimating soil hydraulic properties has limitations, leading to errors in predictions of agricultural and hydrological models that link the processes of evaporation and transpiration at the soil surface through to drainage from the root zone and groundwater recharge. Accurate representation of these processes supports effective water resource management as well as efficient agricultural practices. This study attempted to better constrain the predictive process by evaluating four available methods for estimating soil hydraulic properties.

Soil hydraulic models typically integrate a number of physically based parameters (e.g., water holding capacity) with process-based parameters (e.g., conductivity). These parameters can be derived either directly from soil physical and textural descriptions, in the case of physically based parameters, or through empirical relationships with soil texture in the case of process-based parameters. Large databases of hydraulic parameters have been compiled to facilitate spatial transferability of soil hydraulic models from soil survey data (Cresswell et al., 2006; Schaap et al., 2001). However, soils are heterogeneous at scales of <1 mm to >1 km, leading to difficulty in assigning appropriate parameters to models of soil hydraulics from textural descriptions, which are typically based on a small
number of soil samples or coarsely resolved soil survey information. Preferential flow through macropores contributes substantially to soil hydraulic characteristics (Beven and Germann, 2013; Durner, 1994), resulting in variation of the hydraulic properties of the whole soil column from predictions based on soil texture. Macropore flow can be represented through dual-porosity modeling approaches (Šimůnek et al., 2003). However, these approaches require additional parameterization and input datasets describing macroporosity that are not widely available.

Where measurements of components of the water balance exist, inverse estimation of the hydraulic properties of a whole soil from observations is possible, effectively integrating heterogeneity and macropore flow (Kellners et al., 2005; Naylor et al., 2016; Ritter et al., 2003; Šimůnek et al., 1998). As monitoring networks become denser and more widespread, the addition of well-parameterized points from data inversion will enhance the value of broad soil maps through improved understanding of the spatial variability of soil hydraulic characteristics and scaling of point-based soil data to represent field-scale water fluxes.

Within New Zealand, rapid expansion of the dairy industry has coincided with a 17% increase in irrigated land area since 2005 (Statistics New Zealand, 2013) and an estimated 1900 Gg N yr⁻¹ applied as fertilizer (Ministry for the Environment, 2015) to support additional productivity. This intensification of agricultural land use has generated interest in issues surrounding nutrient and contaminant leaching (Dymond et al., 2013; Jiang et al., 2010). Many of these issues are concentrated on the stony, glacial-alluvial soils of the Canterbury region (Carrick et al., 2013), where variables such as conductivity are known to vary significantly among samples within the same soil type (Webb et al., 2000). Macropore flow has also been observed to be a significant characteristic of these soils (Carrick et al., 2017; Cichota et al., 2016; McLeod et al., 2014). Networks of point-scale measurements of soil drainage (Duncan et al., 2016; White et al., 2003), evapotranspiration (Graham et al., 2016; Pronger et al., 2016), and soil moisture have been deployed in support of efficient agriculture and resource and environmental management efforts. However, there is a particular need for model development to facilitate spatial transfer and upsampling of these point measurements to address management issues at the farm, catchment, and regional scales.

In this study, we compared four methods of soil hydraulic parameterization in a dairy pasture instrumented with an eddy covariance system for measurement of evapotranspiration, drainage lysimeters, and soil moisture sensors. We derived parameters from (i) a multilayer soil description using a pedotransfer function, (ii) a single-layer soil description, (iii) inverse estimation from soil moisture observations, and (iv) inverse estimation from lysimeter drainage. The goal of this comparison was to demonstrate the value of field data networks for improving model parameterizations and provide guidance on the best approach for prediction of each component of soil hydrology: evapotranspiration, drainage, and soil moisture. This method can serve as a model for future efforts to estimate parameter values for different soil hydraulic modeling outcomes.

Methods

Site
This study was conducted in an irrigated pasture in central South Island, New Zealand (43°40′26.61″ S, 171°35′27.63″ E). Vegetation is a mix of perennial ryegrass (*Lolium perenne* L.) and white clover (*Trifolium repens* L.), grazed rotationally by dairy cattle. The Lismore stony silt loam soils at the site are a freely draining, stony glacial alluvium with a silt-loam topsoil texture (Table 1), classified as Pallic Firm Brown (a Typic Dystruustept) (Hewitt, 2010; Soil Survey Staff, 2006). Soils have a volumetric stone content of >50% below the 300-mm depth. During the study period, 1 July 2011 to 15 Mar. 2014, the mean air temperature was 10.5°C and precipitation was 2547 mm. The site also received 532 mm of irrigation, applied by central pivot irrigator in amounts <15 mm d⁻¹ at a typical frequency of 4 to 5 d during the irrigation season (October–April). The total precipitation and irrigation applied during the validation period used in this study (1 Oct. 2012–15 Mar. 2014) was 1807 mm. Potential evapotranspiration for the validation period was 1464 mm.

Field Observations
The field site was instrumented for direct measurement of soil drainage by lysimeter, evapotranspiration by eddy covariance, and soil volumetric water content by soil moisture sensor. Three drainage lysimeters, 500-mm diameter and 700-mm depth, were constructed from undisturbed soil columns following the procedure described by Cameron et al. (1992). Tipping bucket rain

<table>
<thead>
<tr>
<th>Soil depth</th>
<th>Sand</th>
<th>Silt</th>
<th>Clay</th>
<th>Stone content</th>
<th>Bulk density</th>
<th>Field capacity</th>
<th>Wilting point</th>
</tr>
</thead>
<tbody>
<tr>
<td>mm</td>
<td>%</td>
<td>%</td>
<td>%</td>
<td>kg m⁻³</td>
<td>m⁻³ m⁻³</td>
<td>%</td>
<td>%</td>
</tr>
<tr>
<td>0–100</td>
<td>27 ± 2</td>
<td>45 ± 1</td>
<td>28 ± 1</td>
<td>17 ± 3</td>
<td>1060 ± 130</td>
<td>0.27 ± 0.04</td>
<td>0.16 ± 0.01</td>
</tr>
<tr>
<td>100–300</td>
<td>25 ± 1</td>
<td>49 ± 1</td>
<td>27 ± 0</td>
<td>26 ± 3</td>
<td>1430 ± 60</td>
<td>0.28 ± 0.02</td>
<td>0.13 ± 0.01</td>
</tr>
<tr>
<td>300–500</td>
<td>33 ± 4</td>
<td>43 ± 4</td>
<td>25 ± 1</td>
<td>54 ± 4</td>
<td>1860 ± 190</td>
<td>0.21 ± 0.03</td>
<td>0.06 ± 0.01</td>
</tr>
<tr>
<td>500–700</td>
<td>70 ± 5</td>
<td>18 ± 2</td>
<td>13 ± 3</td>
<td>64 ± 2</td>
<td>2010 ± 260</td>
<td>0.11 ± 0.01</td>
<td>0.04 ± 0.00</td>
</tr>
</tbody>
</table>
gauges with 0.2-mm resolution (OSK15180T, OTA) were used to measure the drainage rate. Lysimeters were grazed; however, stock were excluded from standing directly on the lysimeter to prevent damage (for further details, see Duncan et al., 2016). Soil volumetric water content at the 200-mm soil depth was measured immediately outside each lysimeter using a soil moisture sensor (TDT, Acclima Inc.). Processing, filtering, and gap-filling of eddy covariance data used to produce daily estimates of evapotranspiration (ET) were described in detail by Graham et al. (2016).

Precipitation and irrigation were measured by tipping bucket rain gauges installed at ground level, adjacent to the lysimeters. Ancillary climate data (air temperature, relative humidity, wind speed, solar radiation) were also measured at a meteorological station located immediately outside the irrigation footprint area.

**HYDRUS-1D**

Soil drainage, volumetric water content and ET were each simulated using the HYDRUS-1D model, which is based on the Richards equation for unsaturated water flow (Šimůnek et al., 2005):

\[
\frac{\partial \theta}{\partial t} - \frac{\partial}{\partial z} \left[ K \left( \frac{\partial b}{\partial z} - 1 \right) \right] = T
\]

where \(\theta\) is the volumetric water content, \(K\) is hydraulic conductivity, and \(b\) is the matric pressure head at time \(t\) and vertical depth \(z\). Water uptake by roots is accounted for in the sink term \(T\), which is determined by the root water uptake model of Feddes et al. (1978), with root water uptake parameters for pasture from Wesseling et al. (1991). Soil hydraulic parameters within HYDRUS-1D are based on van Genuchten (1980) and Mualem (1976):

\[
S_e(b) = \frac{\theta(b) - \theta_r}{\theta_s - \theta_r} = \left[ \frac{1}{1 + (\alpha b)^n} \right]^m
\]

\[
K(S_e) = K_s S_e^\lambda \left[ 1 - (1 - S_e^{1/m})^m \right]^2
\]

where \(S_e\) is effective saturation and \(\theta_r\), \(\theta_s\), \(\alpha\), \(K_s\), and \(\lambda\) are the residual water content, saturated water content, inverse air entry value, saturated hydraulic conductivity and tortuosity, respectively. The parameters \(n\) and \(m\) are shape parameters correlated by the relationship \(m = 1 - 1/n\).

Within HYDRUS-1D, a vertical soil column was simulated to approximate the field lysimeters—700-mm depth with free drainage at the bottom boundary. Root water uptake was scaled linearly from 1 at the surface to 0 at 700 mm, approximating the root distribution of the pasture crop, which is concentrated in the upper 200 mm of soil (Evans, 1978). An estimate of potential evapotranspiration using the Penman method (Burman and Pochop, 1994) and measured precipitation and irrigation were used as the atmospheric boundary condition. Eddy covariance measurements had previously established similarity between actual and potential evapotranspiration for the irrigated pasture field site (Graham et al., 2016). Partitioning of potential evapotranspiration among plants and soil was implemented within the model with a light extinction function, assuming a leaf area index of 3 m\(^2\) m\(^{-2}\), a median value of pre- and post-grazing leaf area (Korte et al., 1982) because no direct measurements of leaf area were available. This simplification was supported by previous studies that have identified little impact of grazing events on ET in well-watered pasture (Graham et al., 2016; Pronger et al., 2016).

Four methods were used to determine the values of \(\theta_r\), \(\theta_s\), \(\alpha\), \(K_s\), \(n\), and \(\lambda\). The first method involved a four-layer soil description that used a neural-network pedotransfer function (Schaap et al., 2001) to predict parameter values based on sand, silt, and clay fractions, bulk density, the wilting point, and field capacity. These soil attributes were measured at the site for the 0- to 100-, 100- to 300-, 300- to 500-, and 500- to 700-mm soil depths (Table 1). The second method treated the entire 0- to 700-mm soil column as a single layer with a generic silt loam classification, supplied as an option within HYDRUS-1D. Subsequent methods involved inverse parameter estimation from field data. A Marquardt–Levenberg nonlinear parameter optimization approach with an objective function described in detail by Šimůnek et al. (1998) is supported by HYDRUS-1D. Parameter values were optimized within a range of minimum and maximum values (unless left unconstrained): \(\theta_r\) (0–0.15 m\(^3\) m\(^{-3}\)), \(\theta_s\) (0.2–0.6 m\(^3\) m\(^{-3}\)), \(\alpha\) (unconstrained), \(K_s\) (unconstrained), and \(n\) (1–4). Parameter \(\lambda\) was fixed at 0.5, as with the pedotransfer-derived parameter sets. For the third parameterization method, field-measured soil moisture was supplied for inverse parameter estimation. For the fourth method, lysimeter drainage data were supplied. The period 1 July 2011 to 30 Sept. 2012 was used for model spin-up and inverse parameter estimation. Once all hydraulic parameter values were obtained, the model was run with each parameter set for the entire study period (1 July 2011–15 Mar. 2014). However, only a validation period (October 2012–March 2014) was used to assess model performance, avoiding both the effects of model spin-up and overlap with the inverse calibration period. All simulations were initiated during the winter wet season (July) when soil moisture was near field capacity, reducing the impact of initial conditions and minimizing spin-up time (Yang et al., 2011). The initial soil volumetric water content was set to 0.4 m\(^3\) m\(^{-3}\), a value considered close to field capacity.

**Data Analysis**

Because the field observations of volumetric water content and lysimeter drainage were used both for model parameterization and model validation, a separate validation period was used for data analysis (1 Oct. 2012–15 Mar. 2014), which excluded the spin-up and parameter estimation period. The Nash–Sutcliffe efficiency (NSE) and coefficient of determination \((R^2)\) were calculated against field
observations as an indicator of model performance. Further diagnostic statistics were calculated for modeled soil drainage. Local maxima in the drainage time series (≥0.5 mm d⁻¹, to exclude small variations in modeled drainage) were identified, and the total number of peaks was compared with that of the lysimeter time series. Peaks that occurred on the same day in both the measured and modeled time series were counted as exact matches. The lag time between measured precipitation and drainage events was estimated by cross-correlation for lysimeter measurements and individual model parameterizations. Slope and offset differences between measured and modeled data were determined from linear regression.

Results

Method 1: Multilayer Soil Description

Using a multilayer soil description, values of the soil hydraulic parameters derived from a pedotransfer function varied substantially among depths (Table 2). In particular, \(K_s\) decreased from 532 mm d⁻¹ in the surface 100 mm of soil to 41 mm d⁻¹ for the 300- to 500-mm depth layer. Total soil drainage predicted by HYDRUS-1D during the model validation period using this parameterization method was 75% of the mean drainage of three field lysimeters during the same period (421 vs. 560 mm, Table 3). Nash–Sutcliffe model efficiency was −0.07, and the \(R^2\) of the linear relationship between measurement and modeled drainage was 0.09. While 44 drainage peaks were identified in the lysimeter time series, only 20 were identified by the model (Fig. 1). Further, only three peaks occurred on the same day as the lysimeter peak. Cross-correlation analysis indicated that the strongest correlation between precipitation amount and measured lysimeter drainage occurred on the day of the precipitation event (lag = 0, correlation = 0.65). The only other significant cross-correlation was at a lag of 1 d (correlation = 0.43). Modeled drainage showed the strongest correlation with precipitation at a lag of 1 d (correlation = 0.39); however, significant correlations occurred at lag times between 0 and 4 d, indicating that peak timing was delayed compared with lysimeter drainage with the multilayer soil description based parameterization.

Mean predicted soil volumetric water content \((\theta)\) was 0.28 m³ m⁻³, 29% lower than that measured by soil moisture sensor (Table 3).

<table>
<thead>
<tr>
<th>Method</th>
<th>Depth</th>
<th>(\theta_r)</th>
<th>(\theta_s)</th>
<th>(\alpha)</th>
<th>(n)</th>
<th>(K_s)</th>
<th>(l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Four-layer soil description</td>
<td>0–100</td>
<td>0.073</td>
<td>0.509</td>
<td>0.00368</td>
<td>1.32</td>
<td>532.9</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>100–300</td>
<td>0.053</td>
<td>0.408</td>
<td>0.00097</td>
<td>1.40</td>
<td>120.9</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>300–500</td>
<td>0.029</td>
<td>0.300</td>
<td>0.00068</td>
<td>1.45</td>
<td>41.2</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>500–700</td>
<td>0.024</td>
<td>0.259</td>
<td>0.00400</td>
<td>1.35</td>
<td>216</td>
<td>0.5</td>
</tr>
<tr>
<td>One-layer soil description</td>
<td>0–700</td>
<td>0.067</td>
<td>0.450</td>
<td>0.00200</td>
<td>1.41</td>
<td>108</td>
<td>0.5</td>
</tr>
<tr>
<td>Soil moisture inversion</td>
<td>0–700</td>
<td>0.118 ± 0.097</td>
<td>0.489 ± 0.008</td>
<td>0.0042 ± 0.0023</td>
<td>1.07 ± 0.03</td>
<td>570.1 ± 238.3</td>
<td>0.5</td>
</tr>
<tr>
<td>Lysimeter drainage inversion</td>
<td>0–700</td>
<td>0.131 ± 0.048</td>
<td>0.451 ± 0.011</td>
<td>0.0004 ± 0.0001</td>
<td>1.14 ± 0.03</td>
<td>462.3 ± 246.0</td>
<td>0.5</td>
</tr>
</tbody>
</table>

\(\theta_r\), residual water content; \(\theta_s\), saturated water content; \(\alpha\), inverse air-entry value; \(K_s\), saturated hydraulic conductivity; \(l\), tortuosity.

<table>
<thead>
<tr>
<th>Method</th>
<th>Soil drainage</th>
<th>(\theta)</th>
<th>ET</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mm</td>
<td>m³ m⁻³</td>
<td>mm</td>
</tr>
<tr>
<td>Observation</td>
<td>560 ± 85†</td>
<td>0.39 ± 0.01†</td>
<td>1716 (1464)†</td>
</tr>
<tr>
<td>Four-layer soil description</td>
<td>421</td>
<td>0.28</td>
<td>1413</td>
</tr>
<tr>
<td>One-layer soil description</td>
<td>419</td>
<td>0.28</td>
<td>1418</td>
</tr>
<tr>
<td>Soil moisture inversion</td>
<td>521</td>
<td>0.31</td>
<td>1377</td>
</tr>
<tr>
<td>Lysimeter drainage inversion</td>
<td>592</td>
<td>0.31</td>
<td>1202</td>
</tr>
</tbody>
</table>

† Mean (± SE) of three observation points.
‡ Calculated Penman potential evapotranspiration in parentheses.
Fig. 1. Time series comparison of (A) daily observed soil drainage from three lysimeters with (B) drainage simulated by HYDRUS-1D for models parameterized from pedotransfer of a multilayer soil description, (C) a single-layer soil description, (D) inverse parameter estimation from soil moisture data, and (E) inverse estimation from lysimeter drainage during the model validation period (October 2012–March 2014). Daily amounts of precipitation and irrigation ($P+I$) are shown (A). Drainage peaks are highlighted in red to emphasize the enhanced ability of inverse parameter estimation to capture a greater number and timing of peaks.
The NSE for modeled $q$ was $-2.54$, indicating no predictive ability of the model; however, this was primarily due to the downward bias in simulated $q$. The $R^2$ between modeled and observed values was 0.56, suggesting linearity between measurements and model estimates. As well, the simulated $q$ exhibited a seasonal pattern consistent with measurements (Fig. 2).

Total ET was underestimated by the model compared with measurements by eddy covariance (Fig. 3). During the course of the validation period, total modeled ET was 82% of measured ET. However, modeled ET was only 4% less than calculated potential ET.

**Method 2: Single-Layer Soil Description**

Using a single-layer soil description, $K_s$ was estimated as 108 mm d$^{-1}$, which is similar to the median value for all layers predicted by pedotransfer function for the multilayer soil description. Total drainage predicted by this method was similar to that of the multilayer method, 419 mm, although only 13 peaks were detected, only one of which coincided exactly with the timing of lysimeter drainage (Fig. 1). Drainage was delayed relative to antecedent precipitation to a greater extent using this parameterization, with significant lags indicated between 1 and 6 d, the strongest of which occurred at 2 d (correlation $= 0.27$). The NSE for modeled drainage was $-0.10$ using this method, with an $R^2$ of 0.03 for the relationship between observations and predictions (Table 3).

Similar to the multilayer soil description method, the predicted soil volumetric water content was underestimated relative to observations using the single-layer soil description parameter set (Fig. 2). Evapotranspiration was also underestimated by this method, at 82% of the observed total (Fig. 3; Table 3).
Method 3: Inverse Estimation from Soil Moisture

Inverse estimation of the soil hydraulic parameters from soil moisture data resulted primarily in an increased $K_s$ relative to that derived from soil texture, 570 mm d$^{-1}$, although uncertainty, as estimated by the standard error of the nonlinear parameter fit, was high (Table 2). Nonlinear parameter optimization during the calibration period resulted in an $R^2$ of 0.35 for the linear regression between observed and modeled $q$ (see the Supplemental Material for further optimization metrics). As a result of increased conductivity, total drainage during the validation period was increased to within 7% of lysimeter-measured drainage (521 mm, Table 3). Modeled drainage had an NSE of 0.29 and an $R^2$ of 0.38, indicating enhanced ability of this method over soil texture based methods for predicting drainage during validation. The model predicted 27 drainage peaks, seven of which matched the timing of drainage events in the lysimeter time series (Fig. 1). The strongest correlation with antecedent precipitation was at a lag of 1 d (correlation = 0.53). However, significant lags were observed between 0 and 4 d.

Mean $\theta$ was similar to that measured by soil moisture sensor (0.41 and 0.39 m$^3$ m$^{-3}$ for model and observations, respectively). Whereas the soil description based methods resulted primarily in a downward offset bias in $\theta$, the modeled $\theta$ from inverse estimation had a reduced range in water content (Fig. 2), reducing the capability for predicting extreme values of $\theta$.

**Fig. 3.** Comparison of daily observed evapotranspiration ($ET_{obs}$) with (A) evapotranspiration simulated by HYDRUS-1D ($ET_{mod}$) parameterized by pedotransfer from a multilayer soil description, (B) a single-layer soil description, (C) inverse parameter estimation from soil moisture data, and (D) inverse estimation from lysimeter drainage. Slope and offset differences in $ET_{mod}$ are highlighted by the difference between the best-fit linear regression and unity.
Inverse parameter estimates from soil moisture data resulted in further underestimation of the measured ET (Table 3). The modeled ET was 74% of that measured by eddy covariance. The NSE and $R^2$ were likewise reduced relative to soil description based methods.

**Method 4: Inverse Estimation from Lysimeter Drainage**

Similar to inverse estimation from soil moisture data, parameters derived from lysimeter drainage included an enhanced value of $K_v$ (Table 2). Parameter optimization resulted in an $R^2$ of 0.67 for the linear relationship between observed and predicted drainage during the calibration period. Total simulated drainage during the validation period was 592 mm, 6% greater than that measured by lysimeter (Table 3). The model performed similarly for both drainage and soil moisture prediction during the validation period (as determined by NSE and $R^2$) when compared with the model calibrated from soil moisture data. As with soil moisture, the strongest lag between precipitation and drainage was at 1 d (correlation = 0.55), although significant lags were present between 0 and 4 d. Improving on the soil moisture method, the model predicted 36 drainage peaks, nine of which matched the timing of peaks measured by lysimeter.

Inverse estimation from drainage resulted in a substantially reduced range in soil water contents relative to observations of $\theta$ (Fig. 2). The NSE and $R^2$ for the modeled $\theta$ using this method were 0.27 and 0.55, respectively. Evapotranspiration was 70% of that measured by eddy covariance.

**Discussion**

Soil drainage predictions were substantially influenced by the method of parameterization. Soil description based approaches resulted in an overall underestimate of soil drainage amount, fewer drainage peaks, and delayed peak timing relative to measurements by field lysimeter. Low performance metrics for these approaches indicate that efforts to estimate drainage and groundwater recharge may be better served by statistical analysis of drainage data from lysimeter networks. Factors such as spatial heterogeneity, the influence of stones on soil water storage, and macropore flow are not adequately captured by these parameterization methods and a single-porosity modeling approach. Pedotransfer functions used to predict hydraulic parameters generally consider, at most, soil texture, bulk density, field capacity, and the wilting point (Schaap et al., 2001). The underlying development of these functions is typically based on laboratory microcosms (Børgesen et al., 2006; Nemes et al., 2001), thus larger scale heterogeneity and preferential flow pathways are relatively unconsidered.

In this study, inverse parameter estimation from field data improved both total drainage amounts and drainage peak representation. Field measurements incorporate larger volumes of soil (lysimeters are 0.14 m$^3$) and thus may better integrate heterogeneity and processes not represented within the model, such as enhanced conductivity through macropores. Although inverse parameter estimation improved peak representation, modeled drainage continued to arrive primarily on the day following precipitation events, whereas the lysimeter indicated the majority of water arriving on the day of precipitation. This demonstrates the limitations of the single-porosity model used here for simulating rapid flow through macropores while maintaining water retention in the soil matrix, as has been previously shown for Canterbury soils (Jiang et al., 2010). Explicit modeling of macropore flow requires a dual-porosity, dual-permeability approach with additional parameters, thus requiring additional data sources (Simůnek et al., 2003). However, these results demonstrate the potential value of field data based parameterizations for overcoming deficiencies in process representation by a model.

Inverse parameter estimation from soil moisture data performed similarly to inverse estimation with lysimeter data for predicting drainage. Although this result is initially counter-intuitive, because the lysimeter provides a direct measurement of drainage, the soil moisture sensor provides a continuous estimate of water content in the top layer of soil, which is most hydrologically active (e.g., the site of evaporation, infiltration, and root extraction). Thus, soil moisture sensors can be considered a valuable tool for deriving soil hydraulic parameters for modeling and upscaling soil drainage and recharge estimates (Ries et al., 2015; Wang et al., 2016).

In contrast to simulations of soil drainage, which improved in all respects with inverse parameter estimation, there is no clear “best” parameterization method for simulating soil moisture. This highlights the need for use of multiple performance metrics when evaluating model outputs. Soil description based parameterizations primarily resulted in a downward bias in modeled soil moisture, and thus a negative NSE, but maintained a similar seasonal variability to measurements. Inverse estimation from field data resulted in mean soil moisture values within 5% of observations; however, the simulated variation was much smaller. This suggests that parameterizations derived inversely from field data would be better suited to modeling applications that require greater accuracy for longer time periods. Soil description based approaches may perform better for representing short-term variability of soil moisture—as an indicator of drought, for instance. The simple representation of the soil column as a single layer may have contributed to the lower range of simulated soil moisture values using inversion parameterizations. In reality, soil water content typically scales with soil depth. Thus, obtaining parameters that represent the flow of water through the water column but do not incorporate this scaling may overestimate soil water storage, potentially dampening short-term variations in simulated soil moisture. However, this single-layer approach demonstrates how a simple conceptualization can provide useful results when coupled with field data.

Simulations of ET by HYDRUS-1D were 70 to 82% of that measured by eddy covariance during the validation period. The
tendency of the model to underestimate measured ET may be explained, in part, by errors in the input data. During the validation period, measured ET exceeded the calculated potential ET supplied as a boundary condition. However, simulations of ET by HYDRUS-1D were also lower than potential ET, particularly using inversely derived parameter sets. Eddy covariance data at the pasture study site has shown that measured ET is typically linearly related to potential ET, with little evidence of water limitation (Graham et al., 2016). This indicates a degree of water limitation to ET in simulations that is not supported by measurement. Measurements of soil drainage and ET at the site exceed measured precipitation and irrigation by 26% during the model validation period. Weighing lysimeter measurements in a temperate grassland site have previously indicated that tipping bucket rain gauges underestimate low-intensity precipitation events (e.g., fog and dew) (Gebler et al., 2015). As a result, water availability for evapotranspiration may be underestimated. Accumulated errors in the estimation of ET and drainage may contribute to the imbalance. Eddy covariance measurements are typically filtered for conditions under which the assumptions of the method are not met and conditions of instrument failure. One such condition where data are regularly filtered is during precipitation events, when lenses of the open-path gas analyzer are obscured. Thus data gaps, which probably represent conditions of a very limited atmospheric sink for water, must be filled with measured data using regression or look-up table approaches, leading to overestimation of ET. Sources of error in drainage lysimeters may arise from the enhancement of macropore space and other preferential flow pathways by soil disturbance during construction of the lysimeter. Spatial heterogeneity may also contribute to the imbalance among ET, drainage, and applied water. In this study, total precipitation and irrigation were measured at one location with a 130-mm-diameter rain gauge. Soil drainage was measured by three 500-mm-diameter lysimeters within 10 m of each other, while the eddy covariance tower has a dynamic footprint with an approximately 200-m fetch. The large disparity in the spatial representation of each measurement probably contributed to the 26% imbalance between ET and soil drainage and applied water. Despite the observed imbalance, inverse estimation from soil moisture and lysimeter drainage led to model parameterizations that achieved very similar simulations of soil drainage that better represented drainage than soil description based parameterizations. This lends some confidence in our ability to both measure and model drainage.

Conclusions

The choice of the method for estimating soil hydraulic properties can have significant consequences for modeling outcomes. This study investigated four model parameterization methods for an irrigated dairy pasture field site with stony, glacial-alluvial soils. In this case, inverse estimation from field-measured data resulted in parameter sets with an improved capability for representation of total soil drainage and drainage peak timing and shape compared with models parameterized from soil descriptions. This improvement probably resulted from the ability of field measurement based parameter sets to integrate processes not explicitly represented within the model or considered by pedotransfer functions from soil physical properties, such as enhanced hydraulic conductivity due to macropore flow and the impact of stones on storage capacity. Our comparison of model parameterizations based on soil profile description with that of a simplified soil profile with inverse estimation from field data support the value of field measurement networks for parameterizing models of soil drainage from stony soils, which are difficult to both parameterize and model with standard methods. Well-parameterized measurement sites may enhance the value of broad soil maps for spatially upscaling model estimates of drainage and soil moisture when combined with parameter regionalization techniques, supporting efforts to estimate groundwater recharge and nutrient and contaminant leaching. However, the parameterization method will depend largely on the intended use of the model for other outcomes (e.g., ET estimates in support of “smart” irrigation or drought assessment). The approach used in this study can be applied to other settings to determine the most appropriate method for different soils and intended soil hydraulic model applications.

Acknowledgments

This work was funded by the New Zealand Ministry of Business, Innovation and Employment (Contract no. CO1X1006 Watescape) and Environment Canterbury. We thank Craig Mackenzie for the use of his farm. Christian Zammit, Bruce Dudley, Peter Hairsine, and Tim Kane each provided valuable feedback on this manuscript.

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