Efficient Bayesian Inverse Modeling of Water Infiltration in Layered Soils

Hongbei Gao, Jiangjiang Zhang, Cong Liu, Jun Man, Cheng Chen, Laosheng Wu, and Lingzao Zeng*

Modeling water movement in heterogeneous soils, e.g., layered soils, is an essential but challenging task that requires accurate estimation of multiple sets of soil hydraulic parameters. Markov chain Monte Carlo (MCMC) is a popular but computationally expensive method for parameter estimation. An adaptive Gaussian process (GP)-based MCMC method proposed in our previous work presents significant computational efficiency. Nevertheless, its performance was evaluated only for synthetic numerical cases and has not been experimentally validated. Furthermore, its applicability in estimating hydraulic parameters of layered soils is still unknown. In this study, we systematically evaluated the performance of the GP-based MCMC method in estimating the layered soil hydraulic parameters through a water infiltration experiment. It was shown that the proposed method could provide reliable estimations that were very close to those given by the original-model-based MCMC but at a much lower computational cost. The simulated soil water dynamics using the estimated parameters revealed a significant effect of layered heterogeneity on water flow. The lower layer(s) with higher water suction may cause persistent unsaturated status of the upper layer(s) during infiltration.

Abbreviations: GP, Gaussian process; MAP, maximum a posteriori; MCMC, Markov chain Monte Carlo; SWCC, soil water characteristic curve; VGM, van Genuchten–Mualem.

Soil water dynamics play an important role in hydrological cycles (Nakhaei and Šimůnek, 2014). Natural soil profiles present heterogeneity rather than homogeneity in the vadose zone, such as vertical delamination with different textures (Smith and Diekkrüger, 1996). This layered structure in soils is distributed widely in the field along rivers. For example, the lands near the Yellow River and her tributaries have a loamy-sandy soil structure owing to frequent flooding in history (Liu et al., 2015). Water movements in heterogeneous soils exhibit significant variations compared with those in homogeneous soils (Sadeghi et al., 2014). In the past decades, many studies have revealed that an accurate quantification of soil hydraulic processes is essential to regulate limited water resources in agriculture for future benefits (Deng et al., 2006; Evans and Sadler, 2008; Kresović et al., 2016). Because water flow in soils is inevitably impacted by texture and porosity as well as the hydraulic properties of the soil profile (Deng and Zhu, 2015; Gao and Shao, 2015), characterizing the effect of soil heterogeneity on water movement is vital for wise utilization of water resources.

Soil layers with contrasting properties tend to generate interbedded barriers, which may reduce the porous connectivity and subsequently decrease the hydraulic conductivity (Zhang et al., 2012). This blocking has a positive effect by improving the water holding capacity of the upper soil layer(s) (Mantoglou and Gelhar, 1987). Additionally, layer sequences have an obvious impact on water infiltration and drainage (Romano et al., 1998). If soil layers are distributed vertically from fine to coarse, finger flow may appear because of gravity and water repellency in most cases (Ritsema et al., 1993). Conversely, the soil layers distributed from sandy to loamy vertically are beneficial for water storage (Zettl et al., 2011). Ultimately, a heterogeneous soil profile makes it very challenging to predict soil water movement using empirical or semi-empirical hydraulic models because they
have mostly been established based on the homogeneity hypothesis (Kumar et al., 2010; Li et al., 2014).

Several empirical or semi-empirical models considering the effects of heterogeneity have been proposed to describe water movement in soils (Wang et al., 1999; Schneider et al., 2013; Groh et al., 2018). Nevertheless, those models (e.g., the Green–Ampt model or the Philip model) usually require steady-state flow with specified initial and boundary conditions (Prevedello et al., 2009). In practical situations, however, these conditions may be violated and the results may be unsatisfactory (Vereecken et al., 2008). Meanwhile, the uncertainty associated with the estimated hydraulic parameters is unavailable. To this end, more flexible and convenient methods for determining soil hydraulic parameters are needed.

Inverse modeling is drawing increasing attention to the characterization of soil hydraulic properties (Hopmans and Šimůnek, 1999; Vrugt et al., 2008; Zhang et al., 2016b; Xu et al., 2017). In an optimization-based inverse modeling approach, soil hydraulic parameters can be estimated by minimizing the difference between observed and model-predicted values (Tonkin and Doherty, 2005). Because a numerical model can be used, inverse modeling usually accommodates more flexible experimental conditions than empirical or semi-empirical methods, thereby potentially obtaining a more realistic characterization of the soil hydraulic properties (Hopmans et al., 2013; Wöhling and Vrugt, 2011). Additionally, inverse modeling can be used to estimate soil hydraulic properties considering various spatial-temporal scales or structural variations in soil profiles (Dyck and Kachanoski, 2010). It is also a powerful method to avoid many of the problems associated with conventional upscaling methods. In contrast to the conventional approaches requiring information about the spatial distribution of parameters at a small scale, inverse methods are based on observations of state variables and/or fluxes to derive effective model parameters that describe the system behaviors at the scale of interest (Vereecken et al., 2007). However, uncertainties cannot be accurately quantified in the optimization-based inverse approach.

Formulating the inverse problem in a probabilistic framework, Bayesian methods can be used to accurately estimate the unknown parameters and associated uncertainties. As a very popular Bayesian method, Markov chain Monte Carlo (MCMC) requires repeated evaluations of the governing equations to generate posterior parameter samples (Scholer et al., 2012; Zhang et al., 2015; Shi et al., 2014). If the numerical solver is computationally demanding, the computational cost of MCMC simulation will be prohibitive. To address this issue, one promising approach is to replace the original model with an approximated surrogate (Razavi et al., 2012; Asher et al., 2015). Among various surrogates, the Gaussian process (GP) regression has received considerable attention in the past decade (Seeger, 2004). The output of the GP model is described by a normal distribution, with the expression in terms of the mean and variance. In our previous work, an adaptive GP-based MCMC algorithm was proposed to identify a groundwater contaminant source (Zhang et al., 2016a). The numerical simulations showed that this method could provide accuracy comparable to the original-model-based MCMC algorithm but at a much lower computational cost. The adaptive GP-based MCMC method works by iteratively running MCMC and refining the surrogate in the posterior region.

Nevertheless, the applicability of adaptive GP-based MCMC in estimating the hydraulic parameters of layered soils is unknown. Furthermore, this method has not been experimentally validated. In this work, the adaptive GP-based MCMC algorithm was used to estimate the hydraulic parameters of a layered soil using measurements from a water infiltration experiment. The parameter estimation accuracy was then systematically evaluated. The rest of this paper is organized as follows. Below we briefly introduce the experimental and model setups, then present the inverse modeling method based on Gaussian process. To demonstrate the performance of the methods, we provide the detailed results from both laboratory experiments and numerical simulations.

### Materials and Methods

#### Experimental Setup and Data Collection

The water infiltration experiment was conducted on a three-layered soil column consisting of loamy soil and sandy soil. After air drying and grinding, the two soils were sieved using a filter with a 2-mm aperture. Soil particle size distributions were measured using the pipette method (Miller and Miller, 1987). The measurement results of the particle properties are displayed in Table 1.

The tested soils were packed in an acrylic plastic vertical cylinder with 15 cm in diameter and 65 cm in length. The soil bulk densities were 1.4 g cm$^{-3}$ for the loamy soil and 1.65 g cm$^{-3}$ for the sandy soil in the column. During the packing process, two soils were layered alternately in the columns with thickness interval of 20 cm (Fig. 1). The length of the filled soil column was 60 cm. Vertical infiltrations were performed in the soil columns. For comparison, the infiltrations were also conducted in a homogeneous soil column filled with only the loamy soil. A constant water head of 2 cm was maintained above the surface using a Mariotte bottle. The volume of water infiltrated into the soil columns was measured regularly by a ruler stuck on the outside surface of the Mariotte bottle. The movement of the wetting front in the soil columns was also recorded on the cylinder. Volumetric water content was recorded at five points along the column by time-domain reflectometry (Model 5TE, Decagon Devices). Five tensiometers (Model T5x, UMS GmbH) were used to monitor the hydraulic gradient at 10-cm intervals along the columns. The data from all

<table>
<thead>
<tr>
<th>Soil type</th>
<th>No. of samples</th>
<th>Sampling depth (cm)</th>
<th>Particle content</th>
<th>%</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loamy</td>
<td>20</td>
<td>0–20</td>
<td>Sand (&gt;0.05 mm)</td>
<td>8.62</td>
<td>56.47</td>
</tr>
<tr>
<td>Sandy</td>
<td>20</td>
<td>0–20</td>
<td>Silt (0.05–0.002 mm)</td>
<td>10.58</td>
<td>8.08</td>
</tr>
</tbody>
</table>

The tested soils were packed in an acrylic plastic vertical cylinder with 15 cm in diameter and 65 cm in length. The soil bulk densities were 1.4 g cm$^{-3}$ for the loamy soil and 1.65 g cm$^{-3}$ for the sandy soil in the column. During the packing process, two soils were layered alternately in the columns with thickness interval of 20 cm (Fig. 1). The length of the filled soil column was 60 cm. Vertical infiltrations were performed in the soil columns. For comparison, the infiltrations were also conducted in a homogeneous soil column filled with only the loamy soil. A constant water head of 2 cm was maintained above the surface using a Mariotte bottle. The volume of water infiltrated into the soil columns was measured regularly by a ruler stuck on the outside surface of the Mariotte bottle. The movement of the wetting front in the soil columns was also recorded on the cylinder. Volumetric water content was recorded at five points along the column by time-domain reflectometry (Model 5TE, Decagon Devices). Five tensiometers (Model T5x, UMS GmbH) were used to monitor the hydraulic gradient at 10-cm intervals along the columns. The data from all
the probes were recorded using a datalogger (CR1000, Campbell Scientific). Evaporation was avoided by sealing the top of the columns with an upper cap throughout the entire experimental time. The air inlet on the upper cap allowed atmospheric pressure at the soil surface. The bottoms of the soil columns were supported by an acrylic plastic plate with perforations to allow free drainage during infiltration. All operations were performed at 20 to 25°C.

**Model Description**

**Governing Equation of Soil Water Infiltration**

The vertical water movement in the soils can be described using the one-dimensional Richards’ equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(b) \left( \frac{\partial h}{\partial z} + 1 \right) \right]$$  \[1\]

where $\theta$ represents the volumetric water content (cm$^3$ cm$^{-3}$), $t$ is infiltration time (min), $z$ is a spatial coordinate positive upward (cm), $K$ indicates the unsaturated hydraulic conductivity (cm min$^{-1}$), which is a piecewise function of coordinate $z$ to characterize the layered structure (here $z$ is omitted for simplicity), and $h$ is the pressure head (cm). The HYDRUS-1D simulator was used to solve the governing equation combined with prescribed initial and boundary conditions that are given below.

**Soil Hydraulic Properties**

Soil hydraulic properties, including soil water retention, $\theta(b)$, and hydraulic conductivity, $K(b)$, of the soils were parameterized by the van Genuchten–Mualem (VGM) model (van Genuchten, 1980). The soil water retention function is given by

$$\theta(b) = \begin{cases} \theta_s + \frac{\theta_s - \theta_r}{\left[1 + (\alpha b)^{n} \right]^{m}} & \text{if } b < 0 \\ \theta_s & \text{if } b \geq 0 \end{cases}$$  \[2\]

where $\theta_r$ and $\theta_s$ denote the residual and saturated water contents, respectively (cm$^3$ cm$^{-3}$), $\alpha$ is the inverse of the air-entry value (cm$^{-1}$), and $m$ and $n$ represent the pore-size distribution indexes, with $m = 1 - 1/n$. The hydraulic conductivity function is expressed as

$$K(b) = K_s \left[ 1 - \left( S_e^e \right)^{m} \right]^{2}$$  \[3\]

where $K_s$ is the saturated hydraulic conductivity (cm min$^{-1}$), $S_e$ is the effective saturation equal to $(\theta - \theta_r)/\theta_s$, and $l$ is a pore connectivity parameter that is usually set as 0.5.

**Initial and Boundary Conditions**

The soil water potential in the soil column was assumed uniform before water infiltration, i.e., the initial condition of the experiment was given by

$$b(z,0) = b_0, \ (0 \leq z \leq L)$$  \[4\]

where $b_0$ represents the initial pressure head in the soil profile (cm) and $L$ is the length of the soil column (cm).

A constant pressure head of 2 cm was applied to the upper boundary of the soil column during the infiltration process. Meanwhile, the lower boundary was free drainage until the infiltration finished. Thus, the boundary conditions were expressed as

$$b(z,t) = b_0, \ (z = 0, \ t > 0)$$  \[5\]

$$\frac{\partial b}{\partial z} = 0, \ (z = L, \ t > 0)$$  \[6\]

where $b_0 = 2$ cm.

**Inverse Modeling Method**

**Bayesian Parameter Estimation**

Here we briefly introduce the theory of Bayesian parameter estimation. Suppose the unsaturated flow model can be represented by the following compact form:

$$y = F(u)$$  \[7\]

where $y = \{y_1, ..., y_M\}$ signify the model responses with $M$ elements, $F(\cdot)$ is the numerical model, and $u = \{u_1, ..., u_N\}$ represent the soil hydraulic parameters to be estimated. The $M$-elements model responses $y$ correspond to the experimental observations $\hat{y} = \{\hat{y_1}, ..., \hat{y_M}\}$. The prior distribution of $u$ is represented by $p(u)$, which reflects our knowledge about $u$ before the measurement data are obtained. Based on Bayes’ theorem, the posterior distribution of $u$, i.e., $p(u|\hat{y})$, can be given as

$$p(u|\hat{y}) = \frac{p(u)p(\hat{y}|u)}{p(\hat{y})}$$  \[8\]

where $p(\hat{y}) \equiv \mathcal{L}(u|\hat{y})$ is the likelihood function, which measures the mismatch between the model responses $F(u)$ and the
measurements \( \hat{\mathbf{y}} \); \( p(\hat{\mathbf{y}}) \) is the so-called evidence and can be regarded as a normalizing constant. Then, the posterior \( p(\mathbf{u}|\hat{\mathbf{y}}) \) is proportional to the product of the prior and the likelihood, i.e.,

\[
p(\mathbf{u}|\hat{\mathbf{y}}) \propto p(\mathbf{u}) p(\hat{\mathbf{y}}|\mathbf{u})
\]

In this work, the measurement errors are assumed to be independent and normally distributed, \( \mathbf{\sigma} = \{\sigma_1, \ldots, \sigma_M\} \). Then the likelihood function can be expressed as

\[
L(\mathbf{u}|\hat{\mathbf{y}}) = \prod_{i=1}^{M} \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left\{ -\frac{1}{2} \left( \frac{\hat{y}_i - F_i(\mathbf{u})}{\sigma_i} \right)^2 \right\}
\]

where \( F_i(\mathbf{u}) \) is the ith element of model responses \( F(\mathbf{u}) \). In most situations, the analytical form of \( p(\mathbf{u}|\hat{\mathbf{y}}) \) is unavailable. Then MCMC can be used to estimate \( p(\mathbf{u}|\hat{\mathbf{y}}) \) numerically. In this study, we adopted the Differential Evolution Adaptive Metropolis (DREAM(ZS)) algorithm to implement the MCMC simulation, which has been widely used in many different fields, including hydrology and water resources (Vrugt, 2016).

Adaptive Gaussian Process-Based Markov Chain Monte Carlo Simulation

Generally, MCMC requires a large number of model evaluations to fully explore the parameter space, especially when the number of unknown parameters is large. If the numerical model is computationally intensive, the computational cost of MCMC simulation will be prohibitively high. To accelerate the MCMC simulation in parameter inversion, we can use a computationally efficient surrogate to replace the original model. Among various surrogate models, the GP surrogate has been applied extensively to solve many practical problems in the past decade (Rasmussen and Williams, 2006). Gaussian process approximates the input–output relationship of \( \mathbf{F}(\mathbf{u}) \) in a nonparametric Bayesian regression framework. Specifically, the target function \( \mathbf{F}(\mathbf{u}) \) is cast as a Gaussian stochastic process with mean function \( \mu(\mathbf{u}) \) and covariance (kernel) function \( k(\mathbf{u}, \mathbf{u}^*) \):

\[
\mathbf{G}(\mathbf{u}) \sim \text{GP}[\mu(\mathbf{u}), k(\mathbf{u}, \mathbf{u}^*)]
\]

In this study, we chose the zero-mean function \( \mu = 0 \) and the squared exponential covariance function

\[
k(\mathbf{u}, \mathbf{u}^*) = \sigma^2_{\text{GP}} \exp \left\{ -\frac{1}{2} \sum_{i=1}^{M} \frac{(u_i - u_i^*)^2}{l_i^2} \right\}
\]

for the GP surrogate, where \( \mathbf{u} = \{u_1, \ldots, u_M\} \) and \( \mathbf{u}^* = \{u_1^*, \ldots, u_M^*\} \) are two arbitrary parameter samples, and \( \sigma_{\text{GP}} \) and \( l_i \) are the hyper-parameters of GP.

Supposing that \( N_i \) sets of training data, \( \mathbf{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_{N_i}\} \) at design points \( \mathbf{U} = \{\mathbf{u}_1, \ldots, \mathbf{u}_{N_i}\} \) are available, where

\[
\mathbf{y}_i^* = \mathbf{F}(\mathbf{u}_i^*) \quad \text{for} \quad i = 1, \ldots, N_i
\]

we can train the GP surrogate (obtain the optimal hyper-parameters) by minimizing the following objective function:

\[
O = \frac{1}{2} \mathbf{y}^T \mathbf{K}^{-1} \mathbf{y} + \frac{1}{2} \log |\mathbf{K}| + \frac{N_i}{2} \log 2\pi
\]

where \( \mathbf{K} \) is a \( N_i \times N_i \) matrix whose entry at the ith row and jth column is \( k(\mathbf{u}_i, \mathbf{u}_j) \).

Given the optimal hyper-parameters, we can obtain the conditional GP mean \( \mu|_{\mathbf{y}(\mathbf{u})} \) and variance \( \sigma^2|_{\mathbf{y}(\mathbf{u})} \) at an arbitrary parameter sample \( \mathbf{u} \) as

\[
\mu|_{\mathbf{y}(\mathbf{u})} = \mathbf{k}(\mathbf{u}, \mathbf{U}) \mathbf{K}^{-1} \mathbf{y}
\]

\[
\sigma^2|_{\mathbf{y}(\mathbf{u})} = k(\mathbf{u}, \mathbf{u}) - \mathbf{k}(\mathbf{u}, \mathbf{U}) \mathbf{K}^{-1} \mathbf{k}(\mathbf{U}, \mathbf{u})
\]

where \( \mathbf{k}(\mathbf{u}, \mathbf{U}) \) is a \( 1 \times N_i \) vector whose ith element is \( k(\mathbf{u}, \mathbf{u}_i) \), and \( \mathbf{k}(\mathbf{U}, \mathbf{u}) \) is the transpose of \( \mathbf{k}(\mathbf{u}, \mathbf{U}) \).

One advantage of the GP surrogate is that it can be updated conveniently by incorporating new training points provided by the surrogate-based MCMC simulation. This treatment can improve the approximation accuracy of the GP surrogate in a region with high posterior density. Focusing the surrogate accuracy on the posterior region will significantly improve the computational efficiency compared with an approach that guarantees the surrogate accuracy across the whole prior parameter distribution. Specifically, new parameter points drawn from the approximated posterior distribution by surrogate-based MCMC are successively added to the existing training dataset, then the GP surrogate is refined locally by conditioning on the new datasets. The coupled approach of surrogate refinement and surrogate-based MCMC simulation is implemented repeatedly until some predefined criteria are met (Zhang et al., 2016a). The detailed procedure of the adaptive GP-based MCMC algorithm is:

Step 1: Draw \( N_{\text{ini}} \) design points \( \mathbf{U} = \{\mathbf{u}_1, \ldots, \mathbf{u}_{N_{\text{ini}}}\} \) from the prior distribution to generate the initial training dataset \( \mathbf{Y} = \{\mathbf{F}(\mathbf{u}_1), \ldots, \mathbf{F}(\mathbf{u}_{N_{\text{ini}}} )\} \).

Step 2: Build the GP surrogate \( G(\cdot) \) conditioned on the training data \( \mathbf{Y} \).

Step 3: Run the MCMC algorithm with \( G(\cdot) \) to generate samples of the posterior distribution.

Step 4: Randomly choose a small number \( (N_{\text{add}}) \) of parameter samples \( \mathbf{U}_j = \{\mathbf{u}_{i,j}, \ldots, \mathbf{u}_{i,N_{\text{add}}}\} \) from the approximated posterior distribution to generate new training dataset \( \mathbf{Y}_j = \{\mathbf{F}(\mathbf{u}_{i,j}), \ldots, \mathbf{F}(\mathbf{u}_{i,N_{\text{add}}} )\} \) for GP surrogate refinement. Let \( \mathbf{U} = \{\mathbf{U}_j\} \) and \( \mathbf{Y} = \{\mathbf{Y}_j\} \).

Step 5: Repeat Steps 2 to 4 until one of the predefined stop criteria is achieved.

Determining the Prior Distribution of Soil Hydraulic Parameters

Appropriate choices of prior distributions are beneficial in Bayesian estimation. To determine the prior distribution of parameters in the VGM model, some independent experiments were conducted. The saturated soil water content, \( \theta_s \), and residual water content, \( \theta_r \), of the soils were measured using the oven-drying method. In this experiment, 16 air-dried soil cores (5 cm in
diameter and 5 cm in length) at the given bulk density (1.45 g cm\(^{-3}\) for the loamy soil and 1.6 g cm\(^{-3}\) for the sandy soil) of each soil were collected. After weighing, the total of 32 soil cores were saturated with water for 72 h. The constant-head method was applied to the saturated soil cores to measure the saturated hydraulic conductivity, \(K_s\). The saturated soil cores were then dried at 105 °C for >24 h until stabilized in weight. The values of \(a\) and \(\sigma\) were calculated by the differences between the saturated weight and the oven-dried weight and the differences between the air-dried weight and the oven-dried weight, respectively. Additionally, 30 samples of each soil were selected randomly to obtain the soil mechanical compositions. These data were used to determine the prior information of shape parameters \(\alpha\) and \(\eta\) by the ROSETTA program (Schaap and Leij, 2000; Scharnagl et al., 2011). Hypothetically, all the parameters in the VGM follow normal distributions (Russo and Bouton, 1992; Abbaspour et al., 2004; Moreira et al., 2016). Based on these calculated values of \(a\) and \(\sigma\) and the experimental water content \(N\) we empirically drew the prior distribution of the soil hydraulic parameters, we implemented the adaptive GP-based MCMC simulation to infer the model parameters. In the adaptive GP-based MCMC simulation, we empirically drew \(N_{\text{ini}} = 100\) design points, \(U = \{u_1^{\text{ini}}, \ldots, u_{N_{\text{ini}}}^{\text{ini}}\}\), from the prior distribution of model parameters to obtain the initial training data, \(Y = \{F(u_1^{\text{ini}}), \ldots, F(u_{N_{\text{ini}}}^{\text{ini}})\}\). Then we constructed the initial GP surrogate \(G^0\) conditioned on \(Y\) and applied this surrogate to accelerate the MCMC simulation using the DREAM\(_{ZS}\) algorithm (Vrugt, 2016). To accelerate the construction process, those \(N_{\text{ini}}\) design points whose model outputs, \(Y\), are closer to the measurements were recommended to construct the GP surrogate. The comparison between Gaussian likelihood function, i.e., Eq. [10]. From the approximated posterior distribution, we randomly drew \(N_{\text{add}} = 8\) new design points, \(U_{\text{add}} = \{u_1^{\text{add}}, \ldots, u_{N_{\text{add}}}^{\text{add}}\}\), and calculated the corresponding original model outputs, \(Y_{\text{add}} = \{F(u_1^{\text{add}}), \ldots, F(u_{N_{\text{add}}}^{\text{add}})\}\), to obtain the new training data. Based on \(Y = \{Y, Y_{\text{add}}\}\) evaluated at \(U = \{U, U_{\text{add}}\}\), we could train an updated GP surrogate that is more accurate in the high posterior density region than the previous one. The integrated process of surrogate-based MCMC simulation and surrogate refinement was repeated 10 times. Thus, the total number of original model evaluations needed by the adaptive GP-based MCMC simulation is \(N_{\text{total}} = N_{\text{ini}} + 10N_{\text{add}} = 180\).

To verify the estimation accuracy of the surrogate-based approach, we also implemented an MCMC simulation that used only the original model. In this approach, three parallel chains were constructed to sufficiently explore the parameter space. The chains were evolved with long enough length (here the final length of each chain was 10,000, which means the total number of original model evaluations was 30,000). Convergence of the MCMC simulation was monitored with the \(R\) statistics proposed by Gelman and Rubin (1992). As shown in Fig. 2, with about 9000 original model evaluations (i.e., when the length of each chain was about 3000), we could declare a good convergence (i.e., \(R < 1.2\) for all the parameters). Then we used the chain states after convergence to approximate the posterior distribution of model parameters. The results of the original-model-based MCMC simulation served as a reference to check the performance of the surrogate-based approach.

The number of original model evaluations was used as a metric to evaluate the computational cost of the adaptive GP- and original-model-based MCMC simulations. In this work, the average computer processing unit (CPU) time for evaluating the original model simulated with HYDRUS-1D was about 0.84 s. Then the MCMC simulation with the original model required about 7 CPU hours to draw the 30,000 chain states (i.e., \(0.84\times30,000/3600 = 7\) CPU hours). When the original model has a higher complexity and nonlinearity, the running time of the original-model-based MCMC algorithm will be much higher. However, the time to call the GP surrogate once was about 0.002 s, which means that running the GP-based MCMC with 30,000

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Loamy soil</th>
<th>Sandy soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\mu), cm(^{-3})</td>
<td>0.046</td>
<td>0.38</td>
</tr>
<tr>
<td>(\sigma), cm(^{-3})</td>
<td>0.01</td>
<td>0.02</td>
</tr>
<tr>
<td>(\alpha), cm(^{-1})</td>
<td>0.014</td>
<td>0.014</td>
</tr>
<tr>
<td>(\eta)</td>
<td>1.79</td>
<td>1.45</td>
</tr>
<tr>
<td>(K_s), cm min(^{-1})</td>
<td>0.038</td>
<td>2.76</td>
</tr>
</tbody>
</table>

Table 2. Prior distributions of the soil hydraulic parameters including residual and saturated water content (\(\theta_r\) and \(\theta_s\), respectively), saturated hydraulic conductivity (\(K_s\), and shape parameters \(\alpha\) and \(\eta\).
chain samples required about only 1 min. Moreover, the total number of original model evaluations for the adaptive GP-based MCMC simulation was only 180, which constituted a negligible computational time. Thus, the adaptive GP-based MCMC simulation is much more efficient than the original-model-based MCMC simulation.

To verify the accuracy of the GP surrogate, 600 posterior samples were randomly drawn to compare the outputs (volumetric water content) calculated by the final updated GP surrogate and the original model (Fig. 3). The large determination coefficient ($R^2$, 0.9996) and small root mean square error (RMSE, 0.0046 cm$^3$ cm$^{-3}$) indicate the high accuracy of the GP surrogate in the posterior region.

Furthermore, we compare the posterior statistics derived by the adaptive GP- and original-model-based MCMCs in Table 3. These close values of the mean, maximum a posteriori (MAP) and standard deviation (SD) of the parameter estimations indicate the accurate posterior statistics given by the adaptive GP-based MCMC. Meanwhile, Fig. 4 depicts the prior distribution (black curves) and the estimated marginal posterior distributions obtained from the adaptive GP-based (blue dashed curves) and original-model-based MCMCs (red curves) for the 10 unknown parameters. It is clear that the two MCMC approaches could greatly reduce the uncertainties and obtain almost identical posterior distributions. It is also noted that the parameter uncertainties of $\theta_{r,s}$, $\alpha$, and $K_{s,s}$, which are properties of the sandy soil, were not significantly reduced compared with the other parameters. This might have been caused by the relatively lower sensitivity of the measurement data to these three parameters.

In this study, independence was assumed among the different parameters in prior statistics. After assimilating the measurement data, the posterior correlations between some parameters can be observed. Figure 5, shows bivariate scatterplots using posterior samples of the 10 parameters. We found that the correlation existed not only among parameters in a single layer (for example, in the sandy soil layer, $\theta_{r,s}$ was positively correlated with $n$; in the loamy soil layer, $K_{s,s}$ was negatively correlated with $n$), but also among different soil layers (for example, $K_{s,l}$ was positively correlated with $\alpha$). The correlation of parameters for the different soils demonstrates the interaction of soil-water dynamics in the layered soil profile.

The match between the predictions using posterior parameter samples and experimental data is illustrated in Fig. 6, where the shadow areas correspond to the 95% confidence intervals. It

<table>
<thead>
<tr>
<th>Parameter†</th>
<th>GP‡</th>
<th>OM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>MAP</td>
</tr>
<tr>
<td>$\theta_r$, cm$^3$ cm$^{-3}$</td>
<td>0.042</td>
<td>0.043</td>
</tr>
<tr>
<td>$\theta_s$, cm$^3$ cm$^{-3}$</td>
<td>0.368</td>
<td>0.368</td>
</tr>
<tr>
<td>$\alpha$, cm$^{-1}$</td>
<td>0.017</td>
<td>0.017</td>
</tr>
<tr>
<td>$n$</td>
<td>1.835</td>
<td>1.835</td>
</tr>
<tr>
<td>$K_s$, cm min$^{-1}$</td>
<td>0.037</td>
<td>0.037</td>
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<tr>
<td>$\theta_r$, cm$^3$ cm$^{-3}$</td>
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<td>0.019</td>
</tr>
<tr>
<td>$\theta_s$, cm$^3$ cm$^{-3}$</td>
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<td>0.356</td>
</tr>
<tr>
<td>$\alpha$, cm$^{-1}$</td>
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<td>0.340</td>
</tr>
<tr>
<td>$n$</td>
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<td>1.521</td>
</tr>
<tr>
<td>$K_s$, cm min$^{-1}$</td>
<td>2.758</td>
<td>2.758</td>
</tr>
</tbody>
</table>

† $\theta_0$ and $\theta_s$, residual and saturated water content, respectively; $K_s$, saturated hydraulic conductivity; $\alpha$ and $n$, shape parameters.
‡ MAP, maximum a posteriori; 95B<sub>low</sub> and 95B<sub>up</sub>, upper and lower bounds of the 95% confidence interval, respectively.
shows that most of the experimental data can be covered by the 95% confidence intervals, indicating a good uncertainty quantification obtained by the Bayesian estimation.

The soil water characteristic curves (SWCCs) measured by the additional experiments are illustrated in Fig. 7 to further validate the estimated results. Overall, the measured SWCCs of the loamy soil (Fig. 7a) and the sandy soil (Fig. 7b) lie in the center of the posterior realizations. Furthermore, the wider spread of posterior realizations for the sandy layer indicates a larger uncertainty in the parameter estimation. This is in accordance with the results of the posterior distribution shown in Fig. 4, where $\theta_{r,s}$, $\alpha_s$, and $K_{s,s}$ have the smallest uncertainty reduction compared with the other parameters. Additionally, the wide posterior distribution of sandy properties may be associated with the relatively larger input uncertainty.

Fig. 4. Marginal prior distribution (black curves) and the posterior distributions estimated by the original-model (OM)-based Markov chain Monte Carlo (MCMC) (red curves) and the adaptive Gaussian-process (GP)-based MCMC (blue dashed curve) for the residual and saturated water content ($\theta_r$ and $\theta_s$, respectively), saturated hydraulic conductivity ($K_s$), and shape parameters $\alpha$ and $n$. The final subscripts $l$ (a–c) and $s$ (f–j) of the parameters represent the loamy soil and sandy soil, respectively.

Fig. 5. Bivariate scatterplots of posterior (red dots) and prior parameter samples (blue dots) of the residual and saturated water content ($\theta_r$ and $\theta_s$, respectively), saturated hydraulic conductivity ($K_s$), and shape parameters $\alpha$ and $n$. The final subscripts $l$ and $s$ of the parameters represent the loamy soil and sandy soil, respectively.
Hydraulic Process in the Layered Soil

Soil Moisture Content in the Layered Soil

The MAP parameter estimations given by the adaptive GP-based MCMC simulation were used to simulate the hydraulic process in the layered soil. The vertical changes in the observed and simulated volumetric water content of the soil profile are plotted in Fig. 8, where different panels represent different time steps. This illustration clearly again indicates a good fit between the simulation and observation throughout the layered soil profile during the entire infiltrating period. At the layer interfaces (20-cm depth for the loamy–sandy interface and 40-cm depth for the sandy–loamy interface), the simulation could also accurately show the change in soil moisture owing to the soil texture changes (e.g., the red lines in Fig. 8a and 8i).

Another significant difference in the stabilized maximum water content between the loamy layer and sandy layer should be considered. In the loamy soil layers, the maximum soil water content was very close to the predicted saturated water content of 0.37 cm$^3$ cm$^{-3}$. Nevertheless, the maximum water content in the sandy layer was gradually stabilized at 0.23 cm$^3$ cm$^{-3}$, which is significantly lower than its corresponding saturated water content of 0.36 cm$^3$ cm$^{-3}$. This gap in water content signifies the negative influence of stratified structure on water storage of the sandy layer during infiltration. The higher soil water suction in the substratum soil than the sandy soil layer is the most widely accepted interpretation for the vertical infiltration in semi-infinite layered soil columns (Huang et al., 2013; Zettl et al., 2011). Meanwhile, fractured capillaries at the layer interface are an obstacle to exhausting air, which will occupy the soil pores to keep out soil water (Cho, 2016). For soil profiles with a high water table, however, the gap between the stable water content and saturated water content will decrease with the water level (Huang et al., 2011).

A potential influence of the water content gap was the decrease in total soil moisture storage in the layered soil column compared with the uniform soil column during the unsaturated infiltrating process. At the end of the infiltration experiments, water storage in each layer of the stratified column was roughly calculated as 7.35 cm for the upper loamy layer, 4.50 cm for the sandy layer, and 4.10 cm for the bottom loamy layer, amounting to 15.95 cm for the entire column (Fig. 9). The corresponding results for the uniform soil column were 7.20 cm for the upper layer, 6.75 cm for the middle layer, 3.70 cm for the bottom layer, and 17.65 cm for the entire profile. The method for computing the soil water storage has been clearly reported by many researchers and thus is not repeated here (Milly, 1994; Stormont and Morris, 1998; Gao et al., 2016). According to the calculation results, although water storage in the upper layer and bottom layer of the stratified soil profile was higher than those in the homogeneous soil profile, the apparent divergence of water storage between the middle layers of the two soil columns lead to the gap (about 1.70 cm) in total water storage.
storage. For saturated flow in soils, however, it has been proved that a sandy layer existing in the soil profile is helpful to hold more moisture because of fractured capillaries and the air-entry suction of different soil textures (Si et al., 2011). The availabilities of the sandy layer are mainly affected by the layer’s depth and sequence, as well as the textural deviation between adjacent layers (Sreelash et al., 2017).

Distribution of Soil Water Suction in the Layered Soil

The SWCC is used to describe the relationship between soil moisture and soil suction, which are the foundation for calculating the soil water holding capacity. The simulated and measured SWCCs along the vertically layered soil profile at different observation times are presented in Fig. 10. The illustrations clearly show that when the wetting front moved to the first loamy layer (0–20 cm), the vertical distribution of water suction gradually increased (Fig. 10a–10c). However, this did not last when the wetting front was close to the first layer interface (Fig. 10d). The transition was more distinct (Fig. 10e) when the wetting front reached the interface. It should be noted that the pressure head was more sensitive than the water content in reflecting the infiltration process in the layered soil. The simulation results show that the changes in water content occurred around 60 min (Fig. 10e), while the same transformation of pressure head occurred at about 45 min (Fig. 10d). A similar behavior was observed again when the wetting front approached the second layer interface at 40 cm (Fig. 10g).

The projections for simulations (brown lines) and measurements (squares) are also plotted in the $\theta$–$h$ coordinates to show the relationship between soil water content and soil water suction (Fig. 10). The projections of simulations at different times matched well the projected measurements. Particularly, the inflection points in the projections (e.g., Fig. 10i) clearly show the changes in the soil water content–suction relation at the layer interfaces. After the wetting front penetrated the sandy layer, the projected SWCC gap...
between the two layer interfaces gradually diminished with water infiltration. A prediction from this diminishment is the decreased effect of the sandy layer on the soil hydraulic process with increasing moisture. After the water content in the sandy soil layer had stabilized (close to but less than the saturated water content), the capillary water flow at the layer interface became continuous and was helpful to weaken the impediment originating from the difference in texture.

Fig. 10. The vertical distribution of pressure head ($h$) of the layered soil during infiltration. The blue lines signify the simulated pressure head and the brown lines represent the projection of the simulations in the water content ($\theta$)–$h$ coordinate at times of (a–e) 0 to 60 min at 15-min intervals and (f–i) 90 to 270 min at 60-min intervals.

Fig. 11. Vertical distribution of the unsaturated hydraulic conductivity $K(\theta)$ of the layered soil during infiltration. The blue lines signify the simulated $K(\theta)$ and the brown lines represent the projection of the simulations in the $K$–$\theta$ coordinate at times of (a–e) 0 to 60 min at 15-min intervals and (f–i) 90 to 270 min at 60-min intervals.
Simulated Infiltration in the Layered Soil

The unsaturated water conductivity, \( K(\theta) \), in the layered soil profile at different times was calculated to reveal water dynamics in the soil (Fig. 11). The layer properties have a great impact on the unsaturated water conductivity. At the loamy–sandy layer interface (20 cm in the vertical direction), the \( K(\theta) \) presented a significant saltation phenomenon (from 0.036 to 0.028 cm min\(^{-1}\) and then to 0.045 cm min\(^{-1}\)) when the wetting front moved from the loam soil layer into the sand soil layer. This jump in \( K(\theta) \) lasted even when the water content in both the upper and lower layers reached their stabilized values. Once the wetting front moved completely into the second layer (enough water storage in the loamy soil pores before entering), \( K(\theta) \) increased rapidly (from 0.028 to 0.045 cm min\(^{-1}\)) with water content in the sandy soil layer. The main contribution for this increase of \( K(\theta) \) in the sandy layer was caused by more macropores in the sandy soil (Abbaspour et al., 2004). However, when the wetting front was passing through the second layer interface (at 40 cm in depth), a jump and a significant increase in the \( K(\theta) \) value happened. The projections of the simulations in the \( \theta-K \) coordinate can be used to visualize these changes, for example, from 0.001 to 0.012 min\(^{-1}\) at 210 min (Fig. 11h). The range of the jumps was affected by the difference in water suction between the two soil layers around the interface. Although a higher macropore content existed in the sandy soil than in the loamy soil, higher water suction in the lower soil layer drove the wetting front through the layer interface. The rapidly increased water content in the lower loamy soil layer facilitated a higher unsaturated water conductivity than that in the neighboring sandy soil layer.

The measured cumulative infiltration and the infiltration rate were also used to validate the estimated results (Fig. 12). In this illustration, the blue lines indicate the simulated results using the MAP parameter estimations. The gray areas represent the 95% confidence intervals. The comparison (observations vs. the MAP simulations) resulted in \( R^2 = 0.998 \) for cumulative infiltration and \( R^2 = 0.997 \) for infiltration rate, showing that the simulations can well fit the measurements. The RMSE and Nash–Sutcliffe efficiency coefficient (NSE) were also calculated to evaluate the accuracy of the simulations. The NSE values of 0.994 for the cumulative infiltration and 0.999 for the infiltration rate indicate the reliability of the estimated parameters. The RMSE of 0.431 cm for the cumulative infiltration was much lower than the magnitude of measurement errors. In terms of uncertainty quantification, the 95% confidence intervals generally covered all the measurements and became wider with time due to the propagation of uncertainties.

![Fig. 12. Simulated (blue lines) and measured (dots) data for (a) the cumulative infiltration and (b) the infiltration rate. The gray areas indicate the 95% confidence intervals.](image)

**Conclusions**

In this study, the applicability of the adaptive Gaussian process-based MCMC simulation in estimating the layered soil hydraulic parameters was evaluated based on experimental results. Instead of repeatedly solving the original governing equation as in the standard MCMC, a GP surrogate was constructed and adaptively refined in the posterior region during the MCMC sampling. Because it is very cheap to run the GP model, the computational cost of the adaptive GP-based MCMC simulation is rather low. Integrating the experimental observations with Bayesian inverse modeling, we find that:

1. The adaptive GP-based MCMC method can be used to accelerate the inverse modeling of water infiltration in layered soils. The posterior parameter distributions estimated by the adaptive...
3. Quantitative spatial-temporal analyses demonstrated the significant effect of contrasting soil layers on soil water dynamics. The loamy soil layer with a higher water suction capacity is one of the most important reasons for the gap between stabilized water content and saturated water content in the sandy soil layer. This water content gap caused the decrease in water storage in the entire soil profile.

Although GP has seen wide use in many different fields, its application is mainly limited to low-dimensional problems (e.g., with fewer than 50 input parameters). This is because the computational cost of GP construction scales cubically with the number of training data. For a high-dimensional and complex system (e.g., with more than 100 input parameters), a large number of training data are required to train a GP surrogate, which would be extremely time consuming. In this situation, some sampling-free methods, e.g., Bayesian evidential learning (Hermans et al., 2018) or more advanced dimension reduction techniques (Cunningham and Ghahramani, 2015; Ju et al., 2018), should be used.

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References


