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Bayesian analysis of soil water characteristic curve using Markov chain Monte Carlo simulation and its application on soil water infiltration

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ABSTRACT

The soil water characteristic curve (SWCC) is an important property for unsaturated soils and is essential to unsaturated soil engineering analysis. There is significant uncertainty of SWCC obtained by experiment due to the complicated unmodelled influencing factors on SWCC. In this paper, regarding the fitting parameters in Fredlund and Xing (FX) model, Van Genuchten (VG) model, and Gardner model as the random vectors, the uncertainty of SWCC fitting parameters is evaluated using the Bayesian framework. This framework is demonstrated using sandy experimental data with 1,030 records in UNSODA. The posterior distributions of fitting parameters are obtained by the Markov chain Monte Carlo simulation. Different levels of confidence intervals of fitting parameters for FX, VG and Gardner models are obtained intuitively by proposed Bayesian framework. It is found that the confidence interval of the VG model is narrowest, and its uncertainty is the lowest. Different levels of confidence intervals of SWCC with VG model are applied in the one-dimensional vertical soil water filtration. The results demonstrated that the uncertainty in SWCC had significant effects on soil water infiltration.

Keywords: Bayesian framework; Soil water characteristic curve; Uncertainty; Markov chain Monte Carlo; Confidence interval; Soil water infiltration

1. Introduction

The soil water characteristic curve (SWCC) defines the relationship between the water content or degree of saturation and suction of soil which can be used to estimate the unsaturated soil behaviours, such as shear strength, permeability and stress–strain relationships [1–3]. The SWCC represents the water retention ability of the soil at different soil suction and is widely used in geoenvironmental, agricultural and geotechnical engineering [4]. When the SWCC is used to analyze the geotechnical and geoenvironment problems associated with unsaturated zone, the reliability of the input parameters of SWCC directly affects the correctness of the results. It is question about the reliability and predictability of SWCC. It has been recognized that the SWCC is affected by many factors, such as the initial dry intensity [5,6], specimen thickness [7], initial water content [8], grain size distribution [9], stress state [10] and even temperature [11]. The types of soil, test methods, environment factors, including the previously mentioned factors, will make the SWCC have obvious uncertainty. Its predictability is often challenged for researchers.

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In order to predict the SWCC effectively, many mathematical models and fitting methods have been proposed to fit the experimental data of the SWCC [12–15]. The SWCC is commonly expressed using best fit models with several fitting parameters. The parameters of SWCC model depends on the prediction model, fitting method and measure data of the water content versus the soil suction. Since the measurement of the SWCC is always time consuming and expensive due to the equilibrium time for each data point can be very long, only limited experimental data can be obtained. In practice, the fitting parameters in the predict models of SWCC for a given soil are determined by very limited laboratory data using curve fitting technique. It is obvious that the measured data and the curve fitting parameters of SWCC exists high level uncertainty. This uncertainty may lead to uncertainty in the estimated unsaturated soil properties. The uncertainty is mainly caused by the uncertainty of the model structure, uncertainty of input and the uncertainty of the parameters [16,17]. When the model structure can reasonably reflect the soil water characteristics and the measured data have enough accuracy, the uncertainty of the parameters plays a dominant role. Now, more attention has been paid on this kind of uncertainty [18,19]. Parameter values are expressed by probability density function (PDF). Phoon et al. [20] estimated probability of SWCC using a correlated lognormal random vector with two parameters, but it does not involve the confidence interval. The combination of Bayesian approach and the Markov chain Monte Carlo (MCMC) method can solve the problem and quantitatively analyze the uncertainty of parameters.

Bayesian approach can incorporate the prior knowledge into the analysis of current observation data and can estimate the probabilities of the population parameters from the sample data. The uncertainty of any unknown parameters can be described by probability distribution. However, it is very difficult to solve the function, especially for calculating complex problems. The MCMC method which is posterior probability sampling approach based on Bayesian inference can effectively solve the above problems. The MCMC method greatly promotes the application of Bayesian, and develops rapidly. The MCMC has been applied in different research fields, flood frequency analysis [21], consolidation measurements [22]. Bayesian updating analysis of fitting parameters of SWCC based on the measured data is still lacking.

In this paper, a Bayesian framework for prediction of SWCC is established and adopted to evaluate the uncertainty of the fitting parameters for the Fredlund and Xing (FX), Van Genuchten (VG) and Gardner models. The calculation steps are illustrated using sandy data in unsaturated soil hydraulic database (UNSODA), and experimental data within the dry range are required in this paper. The probabilities analysis and parameters uncertainty estimation is performed using the MCMC simulation method which has good efficiency for highly nonlinear problem, with a delayed rejection adaptive metropolis (DRAM) [23] algorithm. The different confidence intervals of uncertainty model parameter for the FX, VG and Gardner models can be obtained. The different confidence intervals of uncertain model parameters can be constructed for one-dimensional vertical soil water filtration analysis.

2. Methodology

2.1. SWCC models

Data associated with the SWCC are commonly plotted as water content or degree of saturation versus the logarithm of soil suction. In order to describe the highly nonlinear SWCC, numerous equations have been proposed for fitting water content or degree of saturation versus soil suction data. Among these equations, the models developed by FX [13], VG [14] and Gardner [12] are some of the most notable ones found in literature. In this paper, these three models are chosen to fit the measured data as shown in Eqs. (1)–(3), respectively, and all models are written in terms of degree of saturation.

FX model [13] can be written as follows:

$$S = \frac{1}{\left(\ln\left(e + \left(\psi/\alpha\right)^{n}\right)\right)^{m}} \tag{1}$$

where α is the fitting parameter related to the air entry value for the soil; n is the fitting parameter related to the pore size distribution of the soil and affects the slope of the SWCC; m is the fitting parameter related to the asymmetry of the model; e is the natural base of logarithms; ψ is the suction; S is the degree of saturation bounded by 0 and 1. The degree of saturation S is the ratio of difference of water content and residual water content to the difference of saturated and residual water contents, as follows:

$$S = \frac{\theta_w - \theta_r}{\theta_s - \theta_r} \tag{2}$$

where θ_w, θ_r, θ_s are the water content, saturated water content and residual water content, respectively. The saturated water content is fixed at experimental value corresponding to zero suction.

VG model [14]

$$S = \frac{1}{\left(1 + \left(\alpha\psi^{n}\right)\right)^{1-n^{-1}}} \tag{3}$$

where α and n are the fitting parameters associated SWCC; ψ is the suction.

Gardner model [12]

$$S = \frac{1}{1 + \alpha\psi^{n}} \tag{4}$$

where α and n are the fitting parameters associated SWCC; ψ is the suction.

2.2. Bayesian framework

Bayesian theory is well suitable for analysis of geotechnical problems, especially when the available information is limited [24]. The unknown parameters can be regarded as a random variable, and described with probability distribution. Based on the Bayesian method, the posterior distribution of parameter ζ is proportional to the product of the likelihood function and the prior distribution function. The Bayes' formula can be written as follows:

$$p(\zeta|D)=\frac{p(D|\zeta)p(\zeta)}{p(D)} \tag{5}$$

where $p(\zeta)$ is the prior probability distribution of the parameters; $p(D|\zeta)$ is the likelihood function; $P(\zeta|D)$ is the posterior distribution of the parameters; $p(D)$ is the normalizing constant to make the PDF valid; ζ is the vector of uncertain input parameters. The prior distribution of parameter ζ and measured data can be integrated using a systematic way.

2.3. Probabilistic analysis

Based on the FX, VG and Gardner models, the uncertainty of fitting parameters is evaluated using the Bayesian framework. The error or difference between the actual performance and the model prediction is defined as the model correction factor ε which can be used to characterize model uncertainty.

$$S_m = S + \varepsilon \tag{6}$$

where S_m is the actual measured degree of saturation; S is the predicted degree of saturation; ε is the model output error which reflects the measurement noise and modelling error and modelled by Gaussian random variable with zero mean and variance σ_ε^2.

The updated posterior PDF of the parameter $\zeta = [\alpha, n, m]$ or $\zeta = [\alpha, n]$ given the data D can be expressed as [25,26]:

$$p(\zeta|D)=c_0 p(\zeta)(2\pi)^{-N/2}\sigma_\varepsilon^{-N}\exp\left[-\frac{N}{2\sigma_\varepsilon^2}J_g(\zeta|D)\right] \tag{7}$$

where c_0 is the normalizing constant; N is the number of measured data points; $p(\zeta)$ is the prior PDF of the model parameters in ζ representing the user's judgment; and $J_g(\zeta|D)$ is the goodness of fit function indicating the level of data fitting and expresses as follows:

$$J_g(\zeta|D)=\frac{1}{N}\sum_{n=1}^{N}\left[S_m(i)-S(\psi;\zeta)\right]^2 \tag{8}$$

where $S_m(i)$ is the measured degree of saturation of i-th record; $S(\psi, \zeta)$ is the corresponding i-th model output of degree of saturation with parameter vector ζ.

The prior PDF of geotechnical parameters is often considered to follow lognormal distributions because fitting parameters in SWCC cannot have negative values [27]. Assuming no correlations between random variables in prior distributions, the prior PDF is described as:

$$p(\zeta)=\prod_{i=1}^{j}\frac{1}{\sqrt{2\pi}\zeta_i\sigma_{\ln\zeta_i}}\exp\left[-\frac{1}{2}\left(\frac{\ln(\zeta_i)-\mu_{\ln\zeta_i}}{\sigma_{\ln\zeta_i}}\right)^2\right] \tag{9}$$

where j is the number of random variables; $\mu_{\ln\zeta i}$ and $\sigma_{\ln\zeta i}$ are the logarithmic mean and standard deviations of the random variable, respectively.

The optimal values of SWCC fitting parameters can be obtained by minimizing the goodness of fit function. The variable $\hat{\sigma}_\varepsilon^2$ for the most probable fitting parameters can be computed by maximizing the posterior PDF and equals to minimum value of the goodness of fit function over all parameter. By solving $\frac{\partial p(\zeta|D)}{\partial\sigma_\varepsilon}=0$, the most probable value of the error variance turns out to be the minimum value of the goodness of fit function.

$$\hat{\sigma}_\varepsilon^2=\min J_g(\zeta|D)=J_g(\hat{\zeta}|D) \tag{10}$$

For large number of data points, the updated PDF of the parameters can be approximated by the Gaussian distribution with mean $\hat{\zeta}$ and covariance $\sum$. The uncertainty of parameters estimated can be represented by the covariance matrix given by the inverse of the Hessian matrix of the function $-\ln p(\zeta|D)$.

$$\sum=\frac{2\hat{\sigma}_\varepsilon^2}{N}\begin{bmatrix}\left.\frac{\partial^2 J_g(\zeta)}{\partial\zeta_1^2}\right|_{\zeta=\hat{\zeta}} & \left.\frac{\partial^2 J_g(\zeta)}{\partial\zeta_1\partial\zeta_2}\right|_{\zeta=\hat{\zeta}} & \cdots & \left.\frac{\partial^2 J_g(\zeta)}{\partial\zeta_1\partial\zeta_k}\right|_{\zeta=\hat{\zeta}} \\ \left.\frac{\partial^2 J_g(\zeta)}{\partial\zeta_2\partial\zeta_1}\right|_{\zeta=\hat{\zeta}} & \left.\frac{\partial^2 J_g(\zeta)}{\partial\zeta_2^2}\right|_{\zeta=\hat{\zeta}} & \cdots & \left.\frac{\partial^2 J_g(\zeta)}{\partial\zeta_2\partial\zeta_k}\right|_{\zeta=\hat{\zeta}} \\ \vdots & \ddots & & \vdots \\ \text{sym} & \cdots & \cdots & \left.\frac{\partial^2 J_g(\zeta)}{\partial\zeta_k^2}\right|_{\zeta=\hat{\zeta}}\end{bmatrix}^{-1} \tag{11}$$

Based on FX, VG and Gardner models, the optimization values of fitting parameters in those models are obtained using the laboratory data for sandy in UNSODA [28]. The UNSODA computer database compiled by U.S. Salinity Laboratory, U.S. Department of Agriculture, contains the soil water retention and unsaturated hydraulic conductivity information of the soils from around the world. There are 780 unsaturated soil samples with the texture of clay, clay loam, loam, loamy sand, sand, sandy clay loam, sandy loam, silt and silt loam in database. In this paper, a total of 80 samples (1,030 suction vs. volumetric water content data pairs) of SWCC data for sandy are selected from the database to demonstrate the probabilistic analysis. Based on the given fitting model, the corresponding model parameters are estimated using the proposed approach. Figs. 1–3 show the posterior PDF of parameters for the FX, VG Gardner models, respectively. Figs. 1(a) and (b) show the corresponding posterior PDF for FX model at $\hat{\alpha}$ = 22.5343 and $\hat{n}$ = 1.9627, respectively. The most probable or optimal

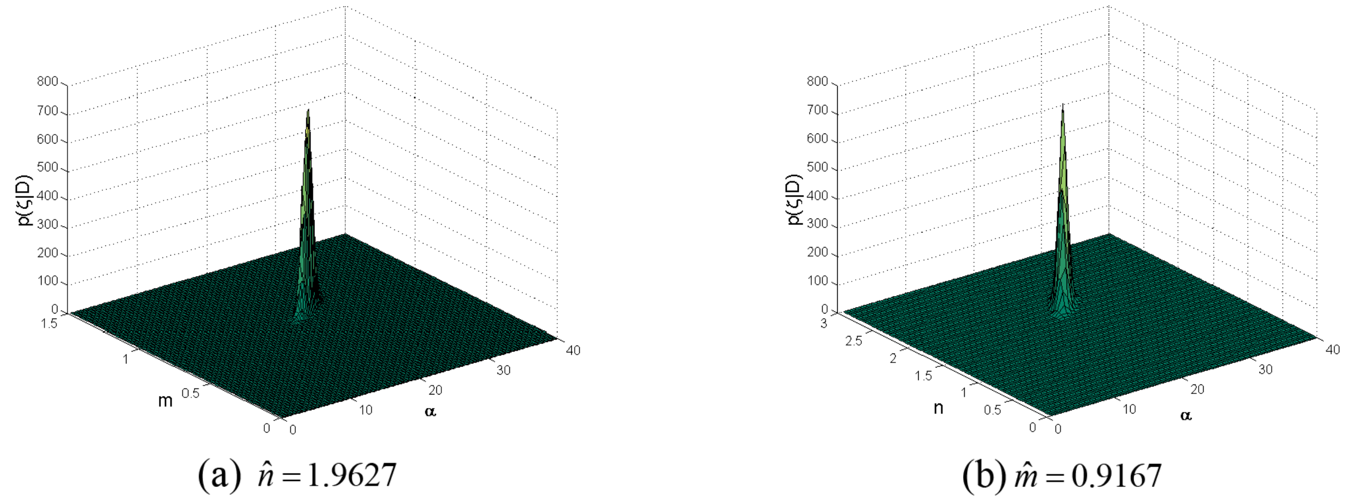

Fig. 1. Posterior PDF of parameters for FX model, (a) $\hat{n}$ = 1.9627 and (b) $\hat{m}$ = 0.9167.

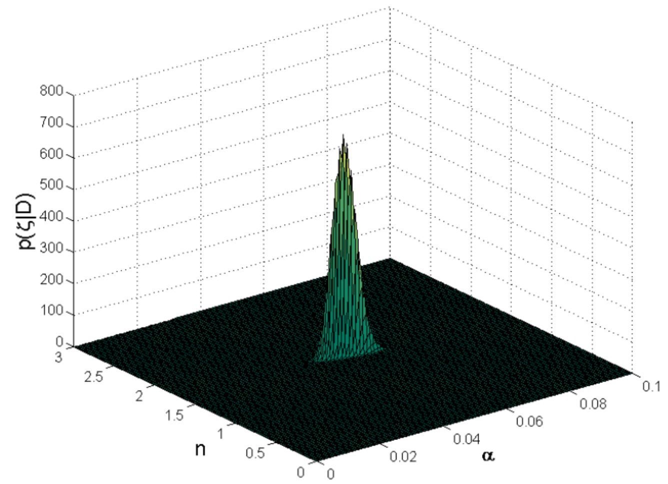

Fig. 2. Posterior PDF of parameters for VG model.

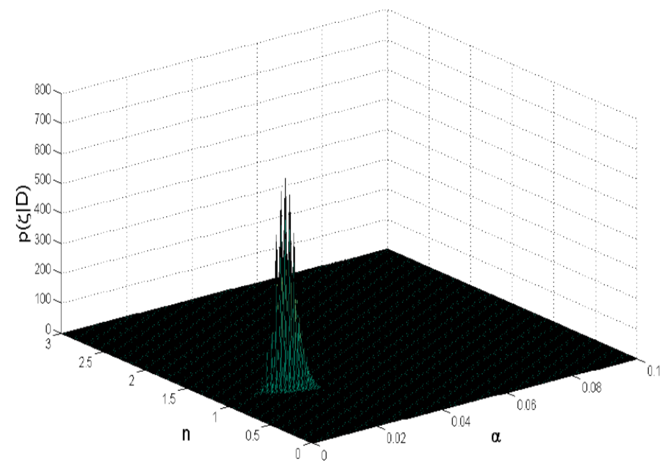

Fig. 3. Posterior PDF of parameters for Gardner model.

fitting parameters corresponding to the maximum value of posterior PDF at $\hat{\alpha}$ = 22.5343, $\hat{n}$ = 1.9627, $\hat{m}$ = 0.9167 for FX model, at $\hat{\alpha}$ = 0.0491, $\hat{n}$ = 1.5929 for VG model and at $\hat{\alpha}$ = 0.0169, $\hat{n}$ = 0.9843 for Gardner model, respectively, as shown by the peaks in Figs. 1–3. Table 1 summarizes statistical information of fitting parameters of SWCC samples for the FX, VG and Gardner models, most probable ($\hat{\alpha}$, $\hat{n}$, $\hat{m}$), mean ($\hat{\alpha}$, $\overline{n}$, $\overline{m}$), standard deviation (σ_α, α_n, σ_m) and output error variance $\hat{\sigma}_\varepsilon^2$.

The SWCC fitted by FX, VG and Gardner models with the most probable parameters from Bayesian analysis and laboratory data for sandy is plotted in Fig. 4. It shows that the modelling error of sandy is large around suction of 10 kPa and beyond suction of 300 kPa. The curve of VG model is between the curves of FX and Gardner models. It is found that the SWCCs obtained by FX, VG and Gardner models with most probable parameter values by Bayesian approach are similar. In other words, the effect of fitting model on the most probable SWCC is small. Especially on straight linear section of curve, the effects of models on the most probable SWCC may be negligible. The line section of the SWCC can be approximately represented with saturated and residual water content and desaturation rate of the SWCC.

2.4. Confidence interval of SWCC

The computational procedure to analyze the confidence interval of SWCC by Bayesian approach involves the following steps:

1. The prior distributions $p(\zeta)$ of the fitting parameters $\zeta = [\alpha, n, m]$ or $\zeta[\alpha, n]$ are set to be lognormal distributions.
2. The likelihood function $p(D|\zeta)$ is determined by measured data.
3. The posterior distribution is used to be the target distribution function, and the random sample generation from posterior distribution is done using DRAM.
4. The samples at the beginning stage are discarded. The remaining samples are used to replace the posterior distribution.
5. The confidence intervals of SWCC are computed.

Bayesian updating can be achieved using Bayesian framework, when conjugate priors are given. The posterior distribution function of input parameters and model predicted response cannot be derived through analytical means.

Table 1
Most probable fitting parameters of SWCC samples

Model	$\hat{\alpha}$	$\bar{\alpha}$	σ_α	$\hat{n}$	$\bar{n}$	σ_n	$\hat{m}$	$\bar{m}$	σ_m	$\hat{\sigma}_\varepsilon^2$
FX	22.5343	22.5525	0.00001	1.9627	1.9650	0.0027	0.9167	0.9171	0.0003	0.0292
VG	0.0491	0.0492	0.000002	1.5929	1.5933	0.0001				0.0300
Gardner	0.0169	0.0169	0.0000002	0.9843	0.9844	0.00005				0.0313

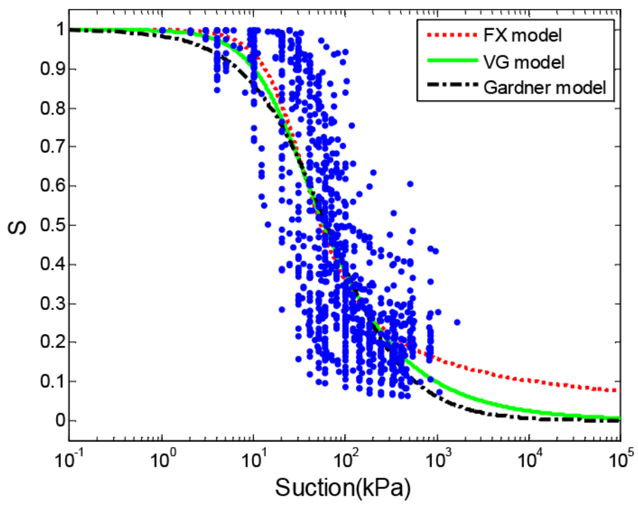

Fig. 4. SWCC of optimal parameters and laboratory data.

Therefore, random sampling methods are needed to generate samples from the posterior distribution function. These posterior distributions are obtained using the MCMC sampling method with DRAM which is an effective random sampling method. The MCMC method can avoid solving the likelihood function and the naturalization constant. The MCMC simulation can maintain adequate sampling density as the number of parameter increases and compute efficiently which has gained popularity in recent years to sample the posterior PDF [18,21]. It can handle efficiently problems with a large number of random variables and is very flexible to any type of prior distribution.

2.5. HYDRUS-1D model

The infiltration processes (vertical flow) in the soil later are further simulated by using HYDRUS-1D model. HYDRUS-1D model was developed by Simunek et al. [29] to simulate the one-dimensional flow of soil water, heat, solute and viruses in variably saturated–unsaturated media (www.hydrus.com). Soil water movement for the experimental situation has been described in the model as follows:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\frac{\partial h}{\partial z}\right] + \frac{\partial K(h)}{\partial z} \tag{12}$$

where θ is the soil volumetric water content; h is the water pressure head; K is the unsaturated hydraulic conductivity; z is the vertical axis depending on the origin of the surface flux.

The VG–Mualem models the variation of $K(h)$ with the soil water content where

$$K(h) = K_s S^l\left[1-\left(1-S^{1/m}\right)^m\right]^2 \tag{13}$$

where $m = 1 - n^{-1}$, l is the empirical parameter of pore connectivity. K_s is the saturated hydraulic conductivity. The SWCC according to VG model is shown in Eq. (3).

We assumed that soil water movement would be restricted to one vertical dimension. The initial soil hydraulic properties used the sandy code 1141 in UNSODA. The dry bulk density is 1.70 g/cm^3, and the saturated water content is 0.302. The initial water content is 0.08. The saturated hydraulic conductivity of the sandy is 38.6 cm/d. The pore connectivity parameter l is assumed equal to an average value (0.5) for many soils. The soil layer is 100 cm. The storage layer is 2 cm deep.

3. Results and discussion

3.1. Results of confidence interval

The SWCC fitting parameters are regarded as a random vector to consider the uncertainty of fitting models. The lab test data of SWCC in the paper are collected from the UNSODA database. The different levels of confidence intervals of SWCC corresponding to FX, VG and Gardner models can be obtained by MCMC simulations. There are 10,000 samples of the SWCC fitting parameters simulated by MCMC method with DRAM for each model. The posterior samples of parameter α in FX model generated by the MCMC method are shown in Fig. 5. As at the beginning stage, the Markov chain does not reach the stationary state, the first 3,000 samples are discarded and not used for posterior statistics inference. The remaining 7,000 pairs of fitting parameters for each model can be generated according to updated PDF of the parameters. Based on the given fitting model, the SWCC for each sample can be obtained and correspond to the updated PDF of the uncertain parameters. Therefore, 7,000 degrees of saturation are generated for a given suction value. After sorting the degree of saturation, the degree of saturation at different percentiles and corresponding fitting parameters can be obtained. This approach is used to evaluate the uncertainty of fitting parameters for FX, VG and Gardner models and can classify its percentile among the database.

The SWCC and fitting parameters associated with different percentiles can be obtained. The fitting parameters of different percentiles SWCC for FX, VG and Gardner models presented in Table 2. Percentiles are used to characterize the confidence interval of the fitting parameters, such as the 50% confidence interval is between 25% (lower bounds) and 75% (upper bound), the 75% confidence interval is between 12.5% (lower bounds) and 87.5% (upper bound), and so on. The upper and lower bounds of SWCC associated with different confidence intervals are evaluated. For FX model, the 95% confidence intervals of the fitting parameter α, n and m are [15.5846, 52.3265], [6.1114, 0.9601] and [2.1579, 0.4761], respectively. For VG model, the 95% confidence interval of the fitting parameter α and n are [0.1261, 0.0270] and [2.1574, 1.3638], respectively. For Gardner model, the 95% confidence interval of the fitting parameter α and n are [0.0806, 0.0088] and [1.1422, 0.6173], respectively. These parameters for confidence intervals of SWCC can be used to conduct the probabilistic analysis of unsaturated geoengineering.

The confidence intervals of SWCC for FX, VG and Gardner models are shown in Figs. 6–8, respectively. The upper and lower bounds of SWCC with different confidence intervals are given. Compared with the FX model and Gardner model, the band of confidence interval of VG model is narrowest. In others words, the VG model has lowest uncertainty or highest reliability for the sandy in UNSODA in the predicted SWCC. The proposed method can be applied to evaluate the SWCC with different fitting model for a given level of confidence.

3.2. Influence of confidence interval on infiltration process

The one-dimensional vertical infiltration process is simulated by HYDRUS-1D software for sandy code 1141 in UNSODA. Using the fitting parameters of VG model with different percentiles in Tables 1 and 2, the soil water content distribution and accumulated infiltration are observed. Fig. 9 shows wetting front depth in sandy simulated by HYDRUS-1D. It can be found that the simulated wetting front depths for the the 50% confidence interval (the 25 and 75 percentiles) and mean are [44.21 cm, 52.58 cm] and 49.50 cm at 800 min, respectively. Fig. 9 shows the cumulative infiltration in sandy simulated HYDRUS-1D. The total cumulative infiltration are (14.578 cm^3, 12.371 cm^3) and 13.880 cm^3 at 800 min for the 50% confidence interval (the 25 and 75 percentiles) and mean, respectively, as shown in Fig. 10. It provides uncertainty estimation of SWCC on one-dimensional vertical infiltration.

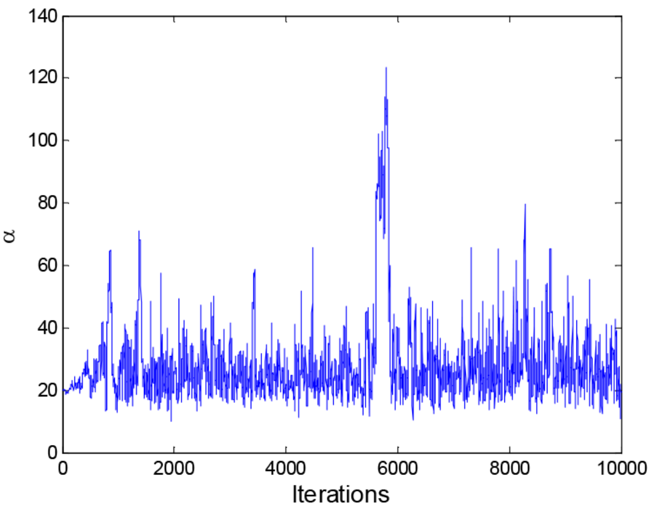

Fig. 5. Posterior samples of parameter α.

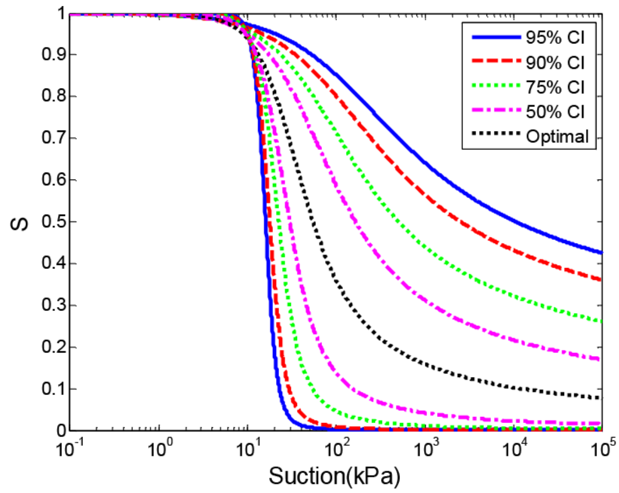

Fig. 6. Confidence intervals of SWCC for FX model.

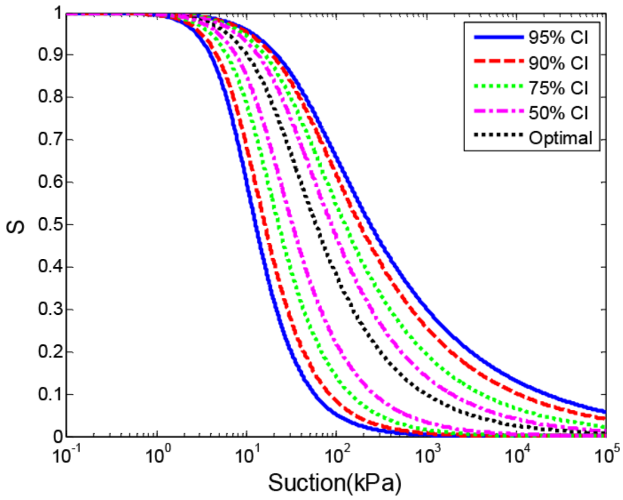

Fig. 7. Confidence intervals of SWCC for VG model.

Table 2
Fitting parameter for different percentiles of SWCC samples

Percentiles		2.5	5	12.5	25	75	87.5	95	97.5
FX	α	15.5846	16.9255	19.0540	21.1731	29.9220	35.7018	44.9811	52.3265
	n	6.1114	4.8370	3.3579	2.5947	1.4490	1.2226	1.0546	0.9601
	m	2.1579	1.8803	1.5721	1.2719	0.7633	0.6378	0.5333	0.4761
VG	α	0.1261	0.1109	0.0835	0.0662	0.0383	0.0335	0.0292	0.0270
	n	2.1574	2.0515	1.9043	1.7958	1.5284	1.4606	1.3974	1.3638
Gardner	α	0.0806	0.0691	0.0533	0.0413	0.0190	0.0142	0.0106	0.0088
	n	1.1422	1.0990	1.0318	0.9609	0.7780	0.7161	0.6569	0.6173

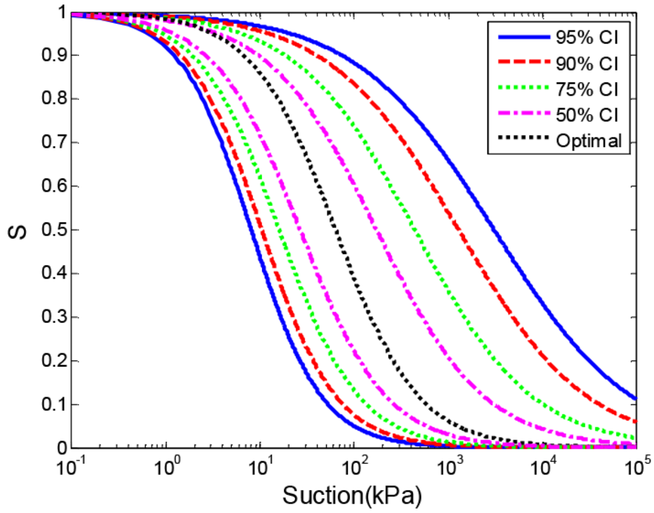

Fig. 8. Confidence intervals of SWCC for Gardner model.

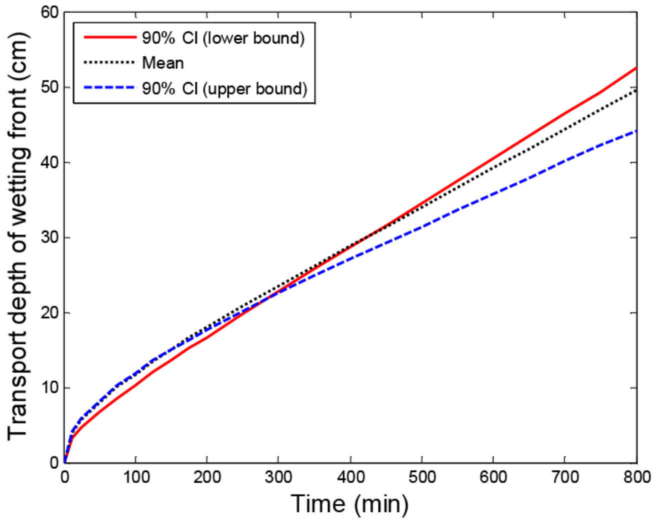

Fig. 9. Transport depth of wetting front.

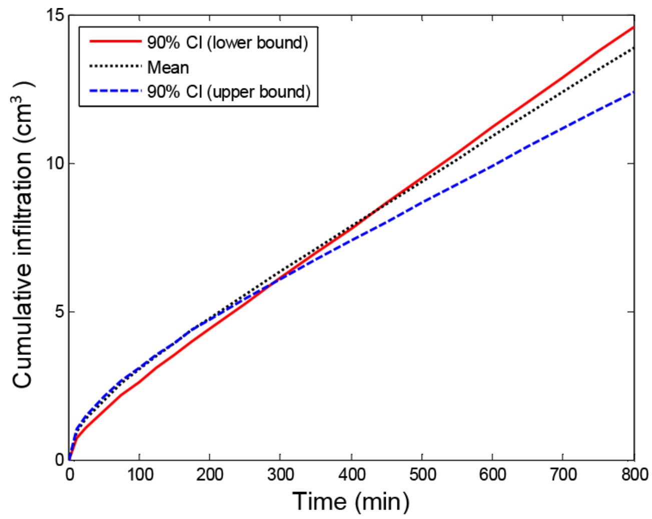

Fig. 10. Cumulative infiltration.

4. Conclusion

In this paper, the updated PDF of the uncertain parameters of FX, VG and Gardner models are evaluated using the Bayesian framework. The proposed approach is demonstrated using experimental data of sandy in UNSODA. The posterior samples of the fitting parameters within SWCC for three different models are generated by MCMC sampling method with DRAM algorithm. The distribution of SWCC can be evaluated, and the percentile among the entire database can be classified using samples of parameters. Different levels of confidence intervals of SWCC are constructed considering the uncertainty of SWCC parameters for sandy by proposed Bayesian approach. It is found that the VG model has the narrowest band of confidence interval for the SWCC which reveals its lowest uncertainty in the predicted SWCC among three fitting models. The approach proposed in this paper can analyze quantitatively the uncertainty, and has good extension. Assuming the VG model as a fitting model of the SWCC, the effect of uncertainty of SWCC on one-dimensional vertical filtration is analyzed. It is found that the uncertainty of SWCC has significant effects on the wetting front depth and cumulative infiltration in the sandy.

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