Proc. of the 8th International Symposium on Geotechnical Safety and Risk (ISGSR)
Edited by Jinsong Huang, D.V. Griffiths, Shui-Hua Jiang, Anna Giacomini and Richard Kelly
 Published by Research Publishing, Singapore.
doi: 10.3850/978-981-18-5182-7_01-010-cd

ISGSR 2022

Probabilistic Experimental Design for Measuring Soil-Water Characteristic Curve Using a Bayesian Approach with One-Stage Optimization

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Abstract: Soil-water characteristic curve (SWCC) is significant to estimate the site-specific unsaturated soil properties (such as unsaturated shear strength and coefficient of permeability) for geotechnical analyses involving unsaturated soils. Determining SWCC can be achieved by fitting data points obtained according to the prescribed experimental scheme, which is specified by the number of measuring points and their corresponding values of the control variable. The number of measuring points is limited since direct measurement of SWCC is often costly and time-consuming. Based on the limited number of measuring points, the estimated SWCC is unavoidably associated with uncertainties, which depends on measurement data obtained from the prescribed experimental scheme. Therefore, it is essential to plan the experimental scheme so as to reduce the uncertainty in the estimated SWCC. This study presented a Bayesian approach, called OBEDO, for probabilistic experimental design optimization of measuring SWCC based on the prior knowledge and information of testing apparatus. The uncertainty in estimated SWCC is quantified and the optimal experimental scheme with the maximum expected utility is determined by Subset Simulation optimization (SSO) in candidate experimental scheme space. The proposed approach is illustrated using an experimental design example given prior knowledge and the information of testing apparatus and is verified based on a set of real loess SWCC data, which were used to generate random experimental schemes to mimic the arbitrary arrangement of measuring points during SWCC testing in practice. Results show that the arbitrary arrangement of measuring points of SWCC testing is hardly superior to the optimal scheme obtained from OBEDO in terms of the expected utility. The proposed OBEDO approach provides a rational tool to optimize the arrangement of measuring points of SWCC test so as to obtain SWCC measurement data with relatively high expected utility for uncertainty reduction.

Keywords: Bayesian approach; Subset Simulation optimization; Probabilistic experiment design; SWCC; Expected utility.

1 Introduction

Soil-water characteristic curve (SWCC) represents the variation of volumetric water content (or effective saturation) with the matrix suction, which is significant to estimate unsaturated soil parameters (e.g., unsaturated shear strength and permeability coefficient) (Lu and Likos, 2004). Only a limited number of SWCC measuring data can be obtained considering that the direct measurement of SWCC is often costly and time-consuming through in-situ or laboratory tests according to some prescribed experimental schemes (i.e., the number of measuring points and their corresponding values of the control variable). The uncertainty of estimating SWCC based on limited data is inevitable, which depends on the data obtained from prescribed experimental schemes and affects the estimation of unsaturated soil parameters and geotechnical reliability analysis (Phoon et al., 2010). Determining an optimal experimental scheme is vital for reducing the uncertainty in SWCC estimated from a limited number of data points.

Experimental design optimization (EDO) provides a rational vehicle to determine the optimal experimental scheme for acquisition of measuring data in a cost-effective way (Sivia and Skilling, 2006). Several EDO methods have been developed in the literature, including conventional experimental design optimization (CEDO) methods based on classical statistics (e.g., Zhu and Gong, 2014) and Bayesian experimental design optimization (BEDO) methods based on Bayesian inference and/or information theory (e.g., Zhang et al., 2015; Ding et al., 2022). Compared with CEDO, the BEDO has an advantage of quantifying various uncertainties (such as inherent variability, measurement error, and model uncertainty), which has been recently applied in geotechnical and geological engineering to design in-situ instrumentation (e.g., Li et al., 2016) and site investigation programs (e.g., Zetterlund et al., 2015). Despite of these previous studies on in-situ monitoring and sampling design, research on applying BEDO to design geotechnical laboratory tests that can be troublesome and time-consuming, e.g., SWCC test, is rare. Ding et al. (2022) proposed a BEDO approach for SWCC testing, which, however, requires to implement the optimization procedure twice at two stages of the experimental design for determining control and additional measuring points, respectively.

This paper presents a one-stage Bayesian experimental design optimization (OBEDO) method for SWCC testing based on Fredlund and Xing (1994) (FX) model, which determines the optimal experimental scheme by implementing a single run of optimization procedure. The proposed method adopts expected utility to quantify the expected value of information provide by SWCC testing. The ancestral sampling and Bayesian method are used to generate simulated data to evaluate the effect of uncertainty of soil parameters. The optimal scheme with maximal expected utility is searched out with Subset Simulation Optimization (SSO), which improves the efficiency of determining the optimal scheme in the design space. This paper starts with description of the proposed OBEDO framework based on FX model, followed by quantifying the expected utility of candidate experimental schemes and optimizing the experimental scheme by maximizing the expected utility using SSO (Li and Ma, 2015). Then, the proposed approach is illustrated using a SWCC experimental design example.

2 One-Stage Bayesian experimental design optimization (OBEDO) framework for measuring SWCC

As shown in Figure 1, the proposed OBEDO framework starts with collecting available prior knowledge (i.e., prevailing SWCC models and typical ranges of its model parameters) on the SWCC of soils concerned before testing and the information of testing apparatus and technique, which are used to determine the design space of candidate experiment schemes. The proposed OBEDO framework is comprised of three steps: determination of the candidate experimental schemes, calculation of the expected utility, $U(E)$, of a possible experimental scheme E that is specified by the number, n, of measuring points, and optimization of the experimental scheme performed by SSO to maximize the $U(E)$. Details of the three steps of the proposed OBEDO framework are provided in the following three sections.

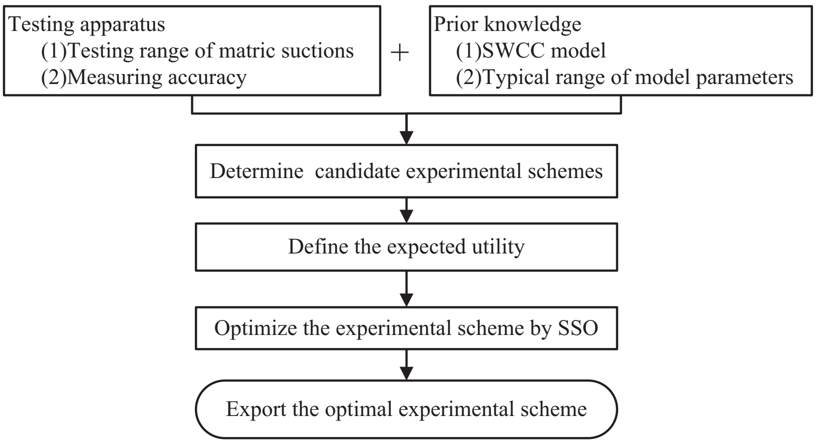

Figure 1. One-stage Bayesian experiment design optimization (OBEDO) framework for measuring SWCC

3 Candidate experimental schemes based on FX model

The trajectory of SWCC can be generally controlled by characteristic matric suction values (such as the air-entry value ψ_b, the matric suction at the inflection point ψ_i, and the matric suction corresponding to the residual water content ψ_r) and their corresponding degrees of saturation. For a given SWCC parametric model, the ψ_b, ψ_i, and ψ_r divide the SWCC into four partitions. There are, at least, four control measuring points selected within the ranges of the matric suction, i.e., $(0,\psi_b]$, $(\psi_b,\psi_i]$, $(\psi_i,\psi_r]$, (ψ_r,ψ_m) to capture the general trajectory of the estimated SWCC and a certain number of additional points selected within the ranges of the matric suction, i.e., $(0,\psi_m)$ to reduce its associated uncertainty. Let n denote the total number of measuring point. Each candidate experimental scheme, E, of SWCC testing is comprised of four control points (i.e., A_1, A_2, A_3, A_4) and (n-4) additional points (i.e., B_1-B_{n-4}), as shown in Figure 2. Nevertheless, during the experimental design stage, the ψ_b, ψ_i, and ψ_r values corresponding to the prescribed SWCC model are unknown. The expected value (i.e., $\bar{\psi}_i$, $\bar{\psi}_b$, and $\bar{\psi}_r$) of ψ_i, ψ_b, ψ_r is adopted to constrain the matric suction range of control point (i.e., A_1, A_2, A_3, A_4), which can be determined using Monte Carlo simulation based on the prior knowledge of SWCC model parameters. Consider, for example, the FX model given below:

$$S_e=\frac{\theta-\theta_r}{\theta_s-\theta_r}=\left[1-\frac{\ln(1+\psi/\psi_r)}{\ln(1+10^6/\psi_r)}\right]\left[\frac{1}{\ln(e+(\psi/a_{fx})^{n_{fx}})}\right]^{m_{fx}} \tag{1}$$

The values of ψ_i, ψ_b, ψ_r corresponding to the FX model satisfy (Zhai et al. 2017)

$$\begin{aligned}&[1-\ln(1+\psi_i/C_r)/\ln(1+10^6/C_r)]\frac{m_{fx}n_{fx}}{a_{fx}}\frac{1}{\ln(e+(\psi_i/a_{fx}))}\frac{1}{e+(\psi_i/a_{fx})^{n_{fx}}}(\psi_i/a_{fx})^{n_{fx}-1}\\&\{\frac{(m_{fx}+1)n_{fx}}{\ln(e+(\psi_i/a_{fx})^{n_{fx}})}\frac{1}{e+(\psi_i/a_{fx})^{n_{fx}}}(\psi_i/a_{fx})^{n_{fx}}+\frac{n_{fx}}{e+(\psi_i/a_{fx})^{n_{fx}}}(\psi_i/a_{fx})^{n_{fx}}-n_{fx}\}+\frac{\psi_i}{\ln(1+10^6/C_r)}(\frac{1}{C_r+\psi_i})^2\\&2\frac{m_{fx}n_{fx}}{\ln(1+10^6/C_r)}\frac{1}{C_r+\psi_i}\frac{1}{\ln(e+(\psi_i/a_{fx})^{n_{fx}})}\frac{1}{e+(\psi_i/a_{fx})^{n_{fx}}}(\psi_i/a_{fx})^{n_{fx}}-\frac{1}{\ln(1+10^6/C_r)}\frac{1}{C_r+\psi_i}=0\end{aligned} \tag{2}$$

$$\psi_b=\psi_i 0.1^{\frac{1-S_{e,i}}{k_1}} \tag{3}$$

$$\psi_r=10^{\frac{S_{e,i}-S'_e+k_1\log(\psi_i)-k_2\log(\psi')}{k_1-k_2}} \tag{4}$$

where a_{fx}, n_{fx} and m_{fx} are the model fitting parameters of FX model; $S_{e,i}$ is an effective degree of saturation corresponding to ψ_i; k_1 is the slope at the inflection point; ψ' is the matric suction where the SWCC starts to drop linearly; S'_e is an effective degree of saturation corresponding to ψ'; and k_2 is the slope at the point (ψ',S'_e). These symbols are illustrated in Figure 3. N_p estimates of ψ_i, ψ_b, and ψ_r can be obtained with the number, N_p, of random samples of a_{fx}, n_{fx} and m_{fx} simulated from their uniform prior distribution through Monte Carlo simulation. Based on the N_p estimates of ψ_i, ψ_b, and ψ_r, their respective mean values (i.e., $\bar{\psi}_i$, $\bar{\psi}_b$, and $\bar{\psi}_r$) are evaluated, with which the matric suction values (i.e., $\psi_{A_1},\psi_{A_2},\psi_{A_3}$, and ψ_{A_4}) of the four control measuring points A1, A2, A3, and A4 are, respectively, assigned within the matric suction ranges $(0,\bar{\psi}_b]$, $(\bar{\psi}_b,\bar{\psi}_i]$, $(\bar{\psi}_i,\bar{\psi}_r]$, and $(\bar{\psi}_r,\psi_m)$. The matric suction values (i.e., ψ_{B_1} - $\psi_{B_{n-4}}$) of n-4 additional measuring points B1-Bn-4 belong to the range, $(0,\psi_m)$, but should not be equal to any values of the four control measuring points A1, A2, A3, A4.

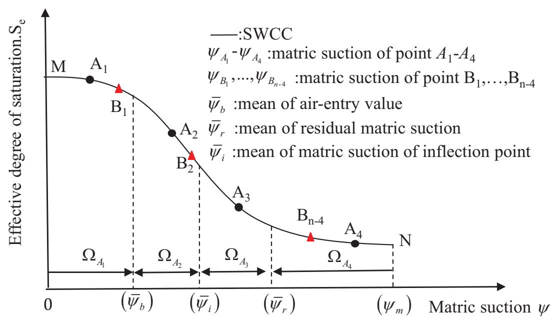

Figure 2. Illustration of control measuring points and additional measuring points

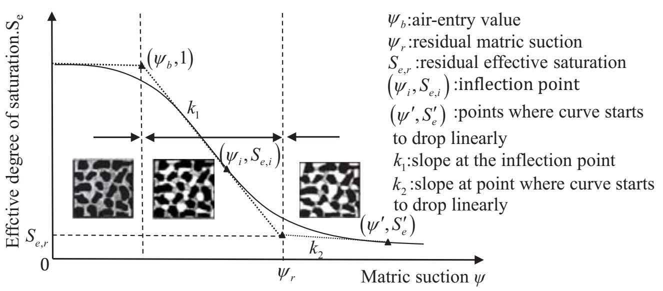

Figure 3. Typical soil-water characteristic curve (Zhai et al. 2017)

Let ψ_h denote the feasible discrete matric suction value, and a set of possible value of ψ_h can be expressed as $\Omega_O=(0{:}\Delta\psi_1{:}\bar{\psi}_b]\cup(\bar{\psi}_b{:}\Delta\psi_2{:}\bar{\psi}_i]\cup(\bar{\psi}_i{:}\Delta\psi_3{:}\bar{\psi}_r]\cup(\bar{\psi}_r{:}\Delta\psi_4{:}\psi_m]$, where $\Delta\psi_1$, $\Delta\psi_2$, $\Delta\psi_3$, $\Delta\psi_4$ are discrete intervals (e.g., the minimum increment of the matric suction that can be applied by the testing apparatus). The above discretization procedure of the matrix suction results in a total of N_O possible values of ψ_h. Assume that N_{A_1}, N_{A_2}, N_{A_3}, and N_{A_4} values of ψ_h in Ω_O fall within $(0,\bar{\psi}_b]$, $(\bar{\psi}_b,\bar{\psi}_i]$, $(\bar{\psi}_i,\bar{\psi}_r]$, and $(\bar{\psi}_r,\psi_m)$, respectively, which constitute the set Ω_{A_1}, Ω_{A_2}, Ω_{A_3}, Ω_{A_4}. The matric suction values (i.e., $\psi_{A_1},\psi_{A_2},\psi_{A_3}$, and ψ_{A_4}) of the control measuring points A1, A2, A3, and A4 satisfied $\psi_{A_1}\in\Omega_{A_1}$, $\psi_{A_2}\in\Omega_{A_2}$, $\psi_{A_3}\in\Omega_{A_3}$, and $\psi_{A_4}\in\Omega_{A_4}$, respectively. Let $\Omega_{B|A}$ denote the set of possible values of the matric suction (i.e., ψ_{B_j}) of each additional measuring point B$_j$ (j=1, 2, …, n-4), which can be written as a set $\Omega_{B|A}=\{\psi_{B_j}\,|\,\psi_{B_j}\in\Omega_O \text{ and } \psi_{B_j}\notin\psi_{A_i}\}$ $(i=1,2,3,4; j=1,2,...,n-4)$. Each set of possible values of $\psi_{A_1}, \psi_{A_2}, \psi_{A_3}$, ψ_{A_4} and ψ_{B_j} (j=1, 2, …, n-4) constitute a candidate experimental scheme E, which can be expressed as

$$E=\left\{\psi_{A_1},\psi_{A_2},\psi_{A_3},\psi_{A_4},\psi_{B_1},\psi_{B_2},\psi_{B_3},...,\psi_{B_{n\text{-}4}}\right\} \tag{5}$$

The optimal experimental scheme is determined by maximizing the expected data worth (i.e., the expected utility $U(E)$) of the SWCC test performed according to candidate experimental schemes using SSO. Calculations of the $U(E)$ of each candidate experimental scheme, E, and its optimization through SSO are provided in the following two sections, respectively.

4 Expected utility of candidate experimental schemes

Consider, for example, a candidate experimental scheme E. The data worth of SWCC test can be quantified by the relative entropy, $R(E)$, that indicates the statistical difference between the updated distribution, $p(\mathbf{\Theta} \mid \mathbf{S_e}, E)$, of SWCC model parameters, $\mathbf{\Theta}$, given a set of newly-obtained data (e.g., values of effective degree of saturation, $\mathbf{S_e}$), obtained according to E and the prior distribution, $p(\mathbf{\Theta} \mid E)$, of $\mathbf{\Theta}$. $R(E)$ can be written as (Sivia and Skilling 2006)

$$R(E)=\int p(\mathbf{\Theta}|\mathbf{S_e},E)\ln[p(\mathbf{\Theta}|\mathbf{S_e},E)/p(\mathbf{\Theta}|E)]\mathrm{d}\mathbf{\Theta} \tag{6}$$

Without the real measurement data at the experimental design stage, the expected utility, $U(E)$, of SWCC measurement data corresponding to E is adopted to quantify the expected worth of data, which is evaluated as (Huan and Marzouk, 2013)

$$U(E)=\int R(E)\,p(\mathbf{S_e}|E)d\mathbf{S_e} \tag{7}$$

where $p(\mathbf{S_e} \mid E)$ is the probability density function (PDF) of $\mathbf{S_e}$ corresponding to E. For the sake of conciseness, more details of the calculation of expected utility are not provided herein and can be referred to Ding et al. (2022) for interested readers.

For a given number of measuring points, the optimal experimental scheme E^* is taken as the scheme with the maximum $U(E)$ among candidate experimental schemes, i.e.,

$$E^*=\arg\max U(E) \tag{8}$$

The next section makes uses of SSO to identify the E^* among candidate experimental schemes.

5 Optimizing the experimental scheme with Subset Simulation

As mentioned in Section 3 entitled "Candidate experimental schemes based on FX model", the number of candidate experimental schemes is equal to $N_{A_1} \cdot N_{A_2} \cdot N_{A_3} \cdot N_{A_4} \cdot C_{N_o-4}^{n-4}$. Identifying the E^* among candidate experimental schemes can be formulated as an optimization problem below:

$$\begin{aligned} &\max_E\ U(E) \\ &s.t.\quad E=\left\{\psi_{A_1},\psi_{A_2},\psi_{A_3},\psi_{A_4},\psi_{B_1},\psi_{B_2},\psi_{B_3},...,\psi_{B_{n\text{-}4}}\right\};\psi_{A_i}\in\Omega_{A_i}\ (i=1,2,...,4);\psi_{B_j}\in\Omega_{D|C}\ (j=1,2,...,n-4)\end{aligned} \tag{9}$$

where the feasible domains (i.e., Ω_{A_i} and $\Omega_{B|A}$) of ψ_{A_i} (i=1, 2, 3, 4) and ψ_{B_j} (j=1, 2, …, n-4) are defined previously in Section 3. In this study, SSO is used to search the E^* in the design space. SSO is a global optimization algorithm that was originally developed from Subset simulation (Li and Ma, 2015). The proposed OBEDO approach makes use of SSO to identify the optimal experimental scheme E^* according to the expected utility, where only one-stage optimization is involved, and returns the one with the maximum expected utility as the E^*, which contains the optimal control and additional measuring points. Hence, the calculation procedure is simplified compared with the two-stage optimization approach.

6 Illustrative example

6.1 Optimal experimental scheme for SWCC testing

In this example, the prior knowledge of FX model parameters are taken as their respective typical ranges $a_{fx} \in (0\text{kPa}, 50\text{kPa}]$, $n_{fx} \in (0,10]$, $m_{fx} \in (0,20]$ and $\sigma_\varepsilon \in (0,1]$, which are consistent with those reported in literature (Tao et al. 2021). Consider, for example, a SWCC testing apparatus with the measured matric suctions range of (0, 2000kPa), which is divided into the matric suction range of $(0,16]$, $(16,26]$, $(26,98]$, and $(98,2000)$ by $\overline{\psi}_b$ =16kPa, $\overline{\psi}_i$ =26kPa, and $\overline{\psi}_r$ =98kPa estimated using the prior knowledge of FX model parameters. Then, the feasible values of the matric suction include Ω_O ={2, 4, 6, …, 14, 16, 18, …, 24, 26, 28, …, 96, 98, 148, 198, …, 1948, 1998} (in kPa) with $\Delta\psi_1$=2kPa, $\Delta\psi_2$=2kPa, $\Delta\psi_3$=2kPa, $\Delta\psi_4$=50kPa.

For consideration of the effect of *n* on the data worth of the candidate experimental scheme, a series of *n* values are considered, including 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 20, and 25. For each of *n* value, the SSO runs with conditional probability p_0=0.1, the maximum number of simulated levels N_s=20, and 2000 samples per level is used to obtain the optimal matric suction values and their corresponding $U(E^*)$ values, as shown in Figure 4. Figure 5 shows the variation of $U(E^*)$ as a function of *n*. It is found that the $U(E^*)$ increases rapidly as *n* is less than 17. The improvement of $U(E^*)$ becomes marginal by adding more measuring points as the *n* is greater than 17. As a result, the optimal number of measuring points is taken as *n*=17 in this example. Correspondingly, the optimal experimental scheme E^* (given *n*=17) is {6, 12, 20, 48, 64, 86, 148, 298, 398, 648, 848, 948, 998, 1048, 1198, 1448, 1598} (in kPa), of which the expected utility (i.e., $U(E^*)$) is 5.27.

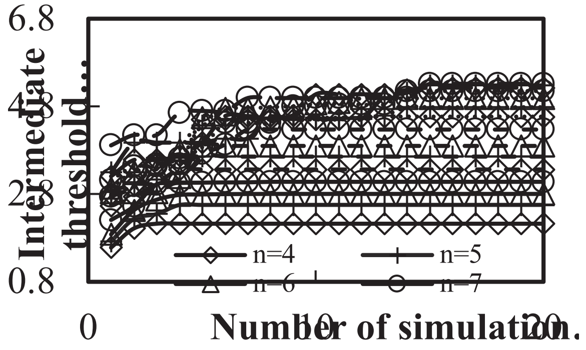

Figure 4. Evolution of SSO for different numbers of measuring points

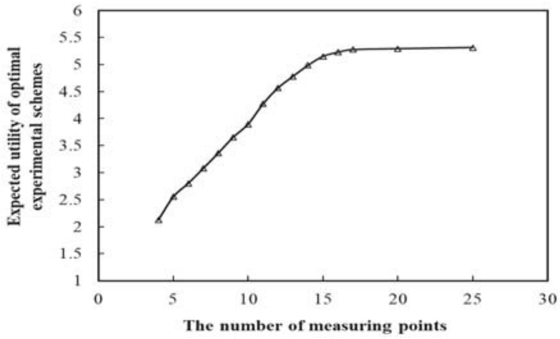

Figure 5. Expected utility with different number of measuring points

6.2 Further illustration with real data of loess

The measured SWCC data of loess that is reported in literature (Punrattanasin et al. 2002; Huang et al. 2009; Chen et al. 2011; Jiao et al. 2016; Wang et al. 2018) is used to verify the effectiveness of proposed method, as shown in Figure 6. The utility (i.e., $R(E)$) that is calculated using Eq.(6) of measured SWCC data obtained from Punrattanasin et al. (2002), Huang et al. (2009), Chen et al. (2011), Jiao et al. (2016), and Wang et al. (2018) are determined as 1.90, 2.06, 0.51, 1.99, and 0.46, respectively. As discussed in subsections 6.1 entitled "Optimal experimental scheme for SWCC testing", the optimal experimental scheme, E^*, obtained from the OBEDO approach and referred to as one-stage Bayesian optimal scheme (OBOS) is {6, 12, 20, 48, 64, 86, 148, 298, 398, 648, 848, 948, 998, 1048, 1198, 1448, 1598} (in kPa), and its expected utility (i.e., 5.27) is superior to the utility of the measured data of loess reported in literature.

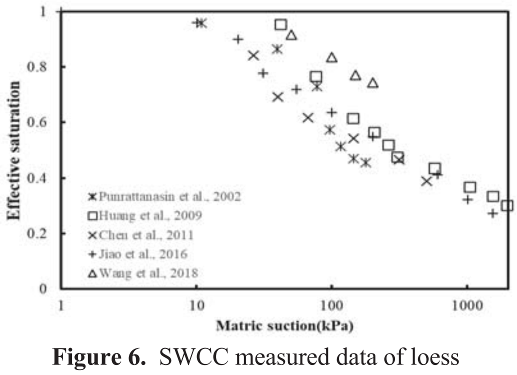

Figure 6. SWCC measured data of loess

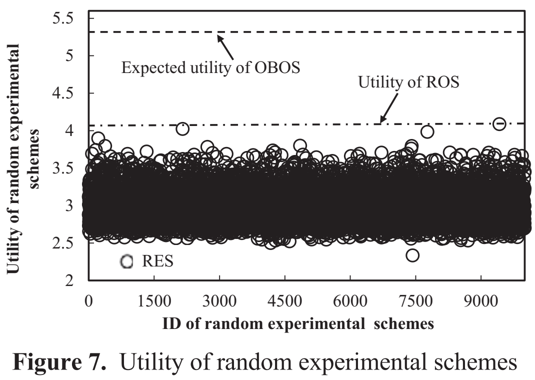

Figure 7. Utility of random experimental schemes

It is worth to point out that the number of measured SWCC data obtained from Punrattanasin et al. (2002), Huang et al. (2009), Chen et al. (2011), Jiao et al. (2016), and Wang et al. (2018) are 7, 10, 6, 9, 4, respectively, which are not consistent with the optimal number (i.e., 17) of SWCC measurements in E^* determined by the proposed method. To enable a consistent comparison, 17 data points are randomly selected from the 36 measurement data points of the loess shown in Figure 6 to mimic the experimental scheme with 17 measuring points, which is referred to random experimental schemes (RES) herein. Figure 7 shows the values of the utility of the 10000 RESs by circles, among which the maximum value is around 4.08 and its corresponding RES is referred to as random optimal scheme (ROS) indicated by the dotted line in Figure 7. The utility of ROS is less than the expected utility (i.e., 5.27) of OBOS obtained from the proposed approach, which demonstrates the effectiveness of proposed OBEDO method.

7 Summary and conclusions

This paper developed a one-stage Bayesian experimental design optimization (OBEDO) approach for determining the optimal experimental scheme of SWCC test using the prior knowledge and the information of testing apparatus. The candidate experimental scheme with the maximum expected utility is identified as the optimal experimental scheme using Subset Simulation optimization (SSO). The proposed OBEDO approach was illustrated using a design example. It was shown that the expected utility of the optimal experimental scheme improves by adding more measurements. Such an improvement becomes marginal as the number of measuring points is sufficiently large (e.g., 17 in the illustrative example). Hence, the optimal number of measuring points can be determined as a trade-off between the improvement of data worth and the commitment involved in testing. The proposed approach was also verified using real loess data. Results showed that the arbitrary arrangement of measuring points of SWCC test is hardly to give the optimal experiment scheme in terms of the expected utility (or values of information). The proposed OBEDO approach provides a rational tool to optimize the arrangement of measuring points of SWCC test based on prior knowledge and the information of testing apparatus so as to obtain SWCC measurement data with relatively high value of information for uncertainty reduction.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (Project Nos. 51879205, 51779189). The financial support is gratefully acknowledged.

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