Evaluation of prediction models applied to the soil-water characteristic curve of ideal materials

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Abstract. The development of theoretical and semi-empirical models to study capillary mechanisms and predict the soil-water characteristic curve (SWCC) generally requires the idealization of pore space and pore water, considering simplifying hypotheses. The study of ideal materials comprised of particles with controlled shape and size allows the evaluation of such simplifying hypotheses and the subsequent generalization to actual soils. In this paper, four theoretical and semi-empirical models for the prediction of the SWCC are applied to the prediction of artificial materials comprised of spherical particles. Nineteen grain-size distribution curves, with varying coefficients of uniformity are considered. The dataset is comprised of materials previously published and additional tests carried out by the authors, under highly controlled conditions. The analyses allowed the evaluation of the effect of grain-size distribution curve and shape of the particles. The limitations and advantages of each prediction model was investigated, and a detailed comparison is presented, guiding future implementations of improved models.

1 Introduction

The soil-water characteristic curve (SWCC) has proved to provide some of the most fundamental and relevant information regarding unsaturated soils' behaviour. For unsaturated soils, the SWCC is as relevant as the grain-size distribution is for saturated soils. Several analyses, behaviour predictions, and properties can be estimated based on SWCC, which make it the key to the implementation of unsaturated soils mechanics. The SWCC is influenced by several retention mechanisms, with capillary retention being the most important. Therefore, the SWCC is influenced by soil mineralogy, grain and pore-size distribution, porosity, surface tension, texture, fabric, particle shape, wetting-drying cycles, the contact angle, entrapped air, among others factors.

The complex retention behaviour of soils has led many researches to develop models to estimate the SWCC using relatively simple properties, such as the grain-size distribution (GSD) and void ratio (e). The works of [1], [5], [2], [6], [7], [3], [8] and [4] are few examples of these methods; however, each model is based on different sets of hypotheses and, therefore, has limitations, providing unreliable results and being applicable to a limited range of soils.

This paper presents a comparison of the performance of the prediction models proposed by [1-4], using glass beads. These artificial materials are nearly spherical, have relatively smooth surface, and present low variability of their properties, making them some of

the simplest material available to evaluate the performance of prediction models.

2 Description of the prediction models

2.1 Arya and Paris [1] and Arya and Dierolf [2]

Arya and Paris [1], observing the similarities between the GSD and the SWCC, developed a model that transforms the grain-size distribution curve into a pore-size distribution (PSD). This model is based on the following simplified hypotheses:

- The bulk density is the same for all fractions;
- The particles of each fraction are assumed spherical with diameter equals to the mean diameter of the fraction;
- The pore volume of each fraction is approximated to the volume of a capillary cylinder with its radius associated to the mean radius of the particles; and
- Hysteresis is neglected.

The first step is to divide the GSD curve in n fractions, each one with a different mean pore diameter. For each fraction, the volume of voids (V_{vi}) is calculated as:

$$V_{vi} = \frac{m_{si}}{\rho_s} e \quad (1)$$

where: $i = 1, 2, 3, \dots, n$; m_{si} is the mass of the i^{th} fraction; ρ_s is the density of the particles; and e is the

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void rate. Also, it is considered that the sum of m_{si} is equal to one, which makes the value of m_{si} equals to its respective percent passing (not accumulated), as represented by the GSD curve.

The accumulated volumetric water content (θ_{vi}) stored up to the fraction i is given by:

$$\theta_{vi} = \sum_{i=1}^n \frac{V_{vi}}{V} = \sum_{i=1}^n V_{vi} \rho_{dry} \quad (2)$$

where: V is the total volume of the soil and ρ_{dry} is the dry density.

For a given particle size range, a mean volumetric water content corresponding to its midpoint can be calculated by:

$$\theta_{vi}^* = \frac{\theta_{vi} + \theta_{vi+1}}{2} \quad (3)$$

Because the authors assumed the particles having a spherical shape and the voids forming a capillary tube, it is possible to describe the particles and volume of voids as:

$$V_{si} = \frac{n_i 4\pi R_i^3}{3} = \frac{m_{si}}{\rho_s} \quad (4)$$

$$V_{vi} = \pi r_i^2 h_i = \frac{m_{si}}{\rho_s} e \quad (5)$$

where for the particles of the i^{th} fraction, V_{si} is its volume; n_i is the number of particles; R_i is the radius the particles. The radius of the cylindric capillary tube is r_i and h_i is the total pore length, for the i^{th} fraction.

Considering the soil having a cubic packing assemblage, the total pore length (h_i) is given by $n_i 2R_i$. However, the authors suggest the adoption of an empirical parameter (α) in order to consider the non-spherical shape of the particles. Therefore, the total pore length (h_i) becomes $n_i^\alpha 2R_i$. Combining the pore length with Equation 5, results in the following equation for r_i :

$$r_i = R_i \sqrt{\frac{4en_i^{1-\alpha}}{6}} \quad (6)$$

Finally, matric suction can be estimated using the Laplace's equation and assuming that the water menisci are spherical caps with a single radius of curvature:

$$(u_a - u_w) = \frac{2T_s}{r_i} \quad (7)$$

where: u_a is the pore-air pressure; and u_w is the pore-water pressure, and T_s is the surface tension.

The parameter α was evaluated by [1] for several soils, with different textures. The authors recommended the adoption of values of α varying from 1.31 to 1.43.

Comparing the predicted curve to laboratory data, reasonable agreement was observed. The overall shape of the SWCC was adequately represented, indicating the strong relationship between the PSD curve estimated from the GSD and the SWCC. The effect of α in the predicted curve was mainly in terms of its overall position. Changes in α produce a translation of the entire SWCC along the matric suction axis. Therefore, it is reasonable to conclude that the empiricism introduced by the α parameter is necessary because the simplifying hypotheses that produced an unrealistic measurement of pore radius.

The limitation of the model proposed by [1] are obviously due to the simplifying hypotheses and due to retention mechanisms, that were neglected. The model neglects the presence of microcracks, root channels, particle aggregation, and non-uniform packing density. In addition, the fact that the pore radius (r_i) is dependent on the number of particles (n_i) is physically untenable, as pointed out by [2]. Despite its limitations, the model proposed by [1] has established a general approach that was followed by many other authors.

To improve Arya and Paris model, [2] proposed an alternative formulation for pore radii. To remove the number of particles (n_i) from the formulation, the authors proposed the introduction of the parameter a new empirical parameter, α^* , defining the total pore length (h_i) as equal to $n_i \alpha^*$. Thus, Equation 6 becomes:

$$r_i = \sqrt{\frac{4eR_i^3}{3\alpha^*}} \quad (8)$$

For the soils tested, the alternative model presented reasonable agreement between the measured and predicted SWCCs. The authors pointed out that the parameter α^* has a narrow range of values. In other words, the modified model proposed by [2] was not as sensitive to the empirical parameter α^* when compared to the sensitivity of the model by [1] with respect to α .

2.2 Aubertin et al. [3]

Basic geotechnical properties of granular and fine-grained materials were used by [3] to predict the SWCC, considering capillarity and particle adhesion. The authors presented an expression (Equation 9) relating the degree of saturation and matric suction diving the retention into adhesive and capillary portions:

$$S = S_c + S_a^* (1 - S_c) \quad (9)$$

where: S_c is the degree of saturation associated with capillary forces; and S_a^* is the degree of saturation caused by adhesion and does not exceed unity at low suctions and defined as:

$$S_a^* = 1 - \langle 1 - S_a \rangle \quad (10)$$

where: $\langle \rangle$ represents the Macauley brackets ($\langle y \rangle = 0.5(y + |y|)$); for $S_a \geq 1$, $S_a^* = 1$, and for $S_a < 1$, $S_a^* = S_a$.

The degrees of saturation associated with capillary forces (Equation 11) and with adhesion (Equation 12) are express as functions of the equivalent capillary rise in the porous medium (h_{co}) and matric suction:

$$S_c = 1 - \left[\left(\frac{h_{co}}{u_a - u_w} \right)^2 + 1 \right]^m \exp \left[-m \left(\frac{h_{co}}{u_a - u_w} \right)^2 \right] \quad (11)$$

$$S_a = a_c C_{(u_a - u_w)} \frac{(h_{co} / \psi_n)^{2/3}}{e^{1/3} ((u_a - u_w) / \psi_n)^{1/6}} \quad (12)$$

$$C_{u_a - u_w} = 1 - \frac{\ln \left(1 + \frac{u_a - u_w}{(u_a - u_w)_r} \right)}{\ln \left(1 + \frac{(u_a - u_w)_0}{(u_a - u_w)_r} \right)} \quad (13)$$

where: m is identified by the authors as the distribution parameter associated with the influence of the PSD curve; a_c is the adhesion coefficient; ψ_n is a normalization parameter; $(u_a - u_w)_r$ is the residual suction; and $(u_a - u_w)_0$ is the suction at complete dryness.

The residual suction $(u_a - u_w)_r$ is calculated according to the material. Parameters from the GSD such as D_{10} (diameter corresponding to 10% passing) and C_U (coefficient of uniformity) are used for granular soils while the liquid limit (w_L) is used for plastic-cohesive materials. Parameters a_c and m were determined from a fitting procedure using experimental data and the basic properties aforementioned.

The authors obtained good agreement between the predicted and measured curves. It was pointed out that there was no clear correlation between the air-entry value and basic geotechnical properties for plastic-cohesive materials. However, for granular materials, the model overestimates of the air-entry value by only about 17%.

Applying the Aubertin et al. [3] model requires caution since some factors such as compaction, hysteresis, volume-change, stress-strain history, multimodal pore size distribution curves and the presence of very coarse particles were not considered. As positive points of the model, the distinction between adhesion and capillary forces can provide more accurate results, mainly for finer soils. In addition, the use of basic geotechnical properties, such as the grain-size distribution curve (D_{10} , C_U), porosity, the density of the particles, and liquid limit (w_L), is an advantage of the method, once it requires only routine laboratory tests to predict the SWCC.

2.3 Wang et al. [4]

Using the van Genuchten's water retention model as basis, [4] developed a model to estimate the SWCC of granular soils based on a semi physical and semi statistical approach. The van Genuchten equation was presented in terms of degree of saturation, as follows:

$$S = \left(1 + \left(\frac{u_a - u_w}{\alpha} \right)^n \right)^{1/n-1} \quad (14)$$

The authors used dimensional analysis to propose the following equation for the variables n and α , which are related to D_{60} and C_U , respectively:

$$n = \frac{C_1}{\log_{10}(C_U)} + 1 \quad (15)$$

$$\alpha = \frac{C_2 \gamma}{D_{60}} \quad (16)$$

A database of 78 granular materials were used to establish the parameters C_1 and C_2 . The obtained values were 1.07 and 12.07, respectively. The validity of the model was tested by estimating the SWCC of six additional soils from the literature. The results showed good agreements between measured and predicted curves.

3 Materials

A dataset of 16 glass beads selected from the literature combined with 3 additional glass beads studies by in the present research project was selected to evaluate the performance of the SWCC prediction models. Table 1 presents the basic information about each material.

Figures 1 and 2 show the grain-size distribution curves of the dataset. Except for the glass beads #1, all materials present low coefficients of uniformity. Notice that the grain-size distribution curves of materials #4 to #11 are defined with only 3 points. In these cases, the GSD is undetermined between 0 and approximately 40% passing. This is a problem for models that use the entire the grain-size distribution curve instead of a fitting equation, namely Arya and Paris [1] and Arya and Dierolf [2]. As consequence, the predictions using these models is also incomplete.

The diameter of the particles of the various glass beads has a relatively wide range, varying by nearly 100 times. The coefficients of uniformity are between 1.04 to 2.19. It is also important to point out that the dataset offers an opportunity to evaluate the effect of porosity, with identical material evaluated at two porosities. The only difference between materials #4 and #5 is the porosity. The same applies to materials #6 and #7, #8 and #9 and #10 and #11.

The tested models do not consider hysteresis effects, they all were developed to predict only the primary drying curves. For this reason, the dataset contains only these types of curves.

Table 1. Basic properties of the dataset.

#	Reference	ρ_s (g/cm ³)	ρ_d (kg/m ³)	n	C_u
1	Authors' results	2.49	1658	0.33	2.19
2		2.46	1589	0.35	1.09
3		2.49	1574	0.37	1.04
4	[9]	2.98	1922	0.36	1.17
5		2.98	1809	0.39	
6		2.98	1931	0.35	1.06
7		2.98	1788	0.40	
8		2.98	1952	0.35	1.07
9		2.98	1836	0.38	
10		2.98	1946	0.35	1.11
11		2.98	1797	0.40	
12	[10]	2.65	1656	0.38	1.14
13		2.65	1606	0.39	2.22
14		2.65	1532	0.42	1.42
15	[11]	2.50	1785	0.29	1.23
16	[4]	2.50	1413	0.44	1.25
17		2.50	1493	0.40	1.25
18		2.50	1468	0.41	1.47
19		2.50	1493	0.40	1.79

4 Results and discussions

Figures 3 to 5 present the results of the prediction exercises for three materials. These materials were selected for presentation because they are representative of the entire dataset. Similar results were obtained for the remaining materials.

The Arya and Paris [1] model overestimated suction for all materials, typically by half to one order of magnitude (i.e., log cycle). In terms of the shape of the SWCC, this model seems to provide better results for materials with relatively higher coefficients of uniformity (Figures 3 to 5).

The results from Arya and Dierolf [2] model are quite similar to those from the Arya and Paris [1] model in terms of the SWCC overall shape, but the first offer grater overestimations of matric suction. This model presented the poorest results among all models. The Arya and Dierolf [2] model has the same limitation of its predecessor regarding the need for grain-size distribution curves with a small number of determination points. This limitation could be overcome by using best-fit equations to represent the GSD, such as those proposed by [12].

The model proposed by Aubertin et al. [3] provided superior predictions when compared with the previous models. The model slightly underestimated matric suctions for some materials, with differences lower than 0.2 of one log cycle. In terms of SWCC slope, the model proposed by Aubertin et al. [3] offered inconsistent

results. For some materials, it provided excellent predictions with slopes nearly identical. However, for 9 out of the 19 glass beads, the predicted SWCC had a noticeably flatter slope. No relationship was observed in terms of the coefficient of uniformity and these prediction imperfections. These relatively minor inconsistencies may be attributed to the complex particle assemblage, not considered by these prediction models.

The model introduced by Wang et al. [4] also provided superior predictions when compared to the models proposed in [1] and [2]. Matric suction was still slightly overestimated for most materials, but the SWCC slopes are relatively accurate. The superior performance of the model by Wang et al. [4] is in part due the broader dataset on which it was based, that specifically includes glass beads.

According to three statistical parameters from the regression analysis shown in Table 1, the best prediction methods were from those proposed by Aubertin et al. [3] and by Wang et al. [4]. Both models are not based only in particle and pores geometry as they include empirical observations that allowed the consideration of the complexity of the soil-water interactions. The models by Aubertin et al. [3] and Wang et al. [4] models use the coefficient of uniformity of the grain-size distribution curve to control the slope of the SWCC. Consequently, they provided the best results.

Fig. 1. Grain-size distribution curve of materials #1 to #11.

Fig. 2. Grain-size distribution curve of materials #12 to #19.

Fig. 3. Measured and predicted SWCC of material #1.

Fig. 4. Measured and predicted SWCC of material #5.

Fig. 5. Measured and predicted SWCC of material #19.

Table 2. Average parameters obtained from the regression analysis of the dataset.

Model	RMSE	SSE	R ²
Arya and Paris [1]	0.178	0.477	-0.819
Arya and Dierolf [2]	0.217	0.675	-1.548
Aubertin et al. [3]	0.071	0.075	0.698
Wang et al. [4]	0.077	0.092	0.567

3 Conclusions

Some of the main models available to predict the SWCC are based on simplifications of the particle-pore geometry. Therefore, the investigation of the behaviour of such models using simple ideal materials allows a better understanding of the performance of these models. Glass beads are some of the most simple material that may be used in the calibration and evaluation of prediction models.

Four predictions models, [1 – 4] were evaluated using a dataset comprised of 19 glass beads varying in grain-size distribution, porosity and density of particles. Regression analysis using RMSE, SSE and R² were performed to measure the goodness of fit of the models.

The Arya and Paris [1] and the Arya and Dierolf [2] models presented similar behaviour of overestimating suction. Despite the fact that the Arya and Dierolf [2] model is supposed to be an improvement of Arya and Paris [1] model, the first earlier original model was superior.

The models that considers the shape of the grain-size distribution curve provided the best results [3 – 4]. Both models were capable of reproducing adequately the air-entry value and the slope of the SWCC. The regression analysis indicates the model by Wang et al. [4] is

particularly accurate, since it has been developed considering glass beads and sands.

A more comprehensive investigation using sands and considering its irregular particle geometry is necessary to test and the performance of the models and to expand the analyses to a broader dataset.

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