Micromechanics modeling on the prediction of soil-water characteristic curves

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February 20, 2023

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Micromechanics modeling on the prediction of soil-water characteristic curves

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Abstract: The soil-water characteristic curve (SWCC) plays an important role in the prediction of soil performance. To predict the water film thickness on the surface of grains, a chemical model is proposed by considering the effects of van der Waals forces and electric double-layer forces. Then a liquid bridge model is proposed to predict the relationship between water content and matric suction of two contacted spherical grains. By studying the microstructure and incorporating the liquid bridge model into the representative volume element of soils, the SWCC of soils is derived and the volume of water films corresponds to the residual water content. The contact angle hysteresis is considered to capture the SWCC hysteresis, and the concept of equivalent grain radius is proposed to consider the effect of grain-size distribution. By comparing test data and model predictions, it is found that the proposed model captures the SWCC of soils well. Model predictions also reveal a new swelling and shrinkage mechanisms of expansive soils. At a low water content, the suction is huge for fine grains, and this causes the shrinkage of expansive soils. When the water content approaches to be saturated, the matric suction is negative and it forces the separation of contacted grains. This contributes to the swelling of expansive soils. It also reveals that the change of SWCC after wetting-drying cycles arises from the microstructure change of soils. At a given water content, the matric suction decreases with the increase of porosity.

Key Points: Contact angle hysteresis; Microstructure; SWCC; Unsaturated soils; Water film.

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1. Introduction

The soil-water characteristic curve (SWCC) is used to describe the relationship between the water content and matric suction in unsaturated soils, which is composed of soil solids, water, air and air-water interfaces (Fredlund & Rahardjo, 1993). The SWCC affects soil performance considerably, like the shear strength (Fredlund et al., 1996), aqueous diffusion (Lim et al., 1998), hydraulic conductivity (Mualem, 1976) and deformation (Kim et al., 2018). At a given water content, the matric suction during drying process is higher than that during wetting process. Thus, SWCCs are hysteretic and include drying SWCCs and wetting SWCCs. The difference between these two types of curves mainly arise from the contact angle hysteresis (the advancing contact angle of liquid on solid surfaces is larger the receding contact angle) (Gao & McCarthy, 2006; Likos & Jaafar, 2013; Mampallil, 2014). Direct measurement of SWCCs is expensive and time-consuming, so researchers prefer to propose models to predict SWCCs and use the measured data to verify their models.

There are three different approaches on the prediction of SWCC, namely empirical methods, domain methods, and theoretical methods. The first approach is the most popular and many empirical models have been proposed. In some empirical models (Feng & Fredlund, 1999; Fredlund & Xing, 1994; Karube & Kawai, 2001; Kawai et al., 2020; Kong et al., 2018), SWCC equations containing empirical parameters were proposed and using these equations, the matric suction can be obtained directly once the water content is known. Other empirical models were proposed based on machine learning (Baghbani et al., 2022; Li & Vanapalli, 2022a, 2022b) and pedo-transfer functions (Bayat et al., 2019; Wang et al., 2017), so SWCC could be predicted from some easy-to-measure soil properties, like the grain-size distribution (Fredlund et al., 2002), pore-size distribution (Simms & Yanful, 2002) and density of soils (Wijaya & Leong, 2017). However, the main drawback of the empirical approach is that it does not have a sound theoretical basis, and has substantial uncertainty and variability. The accuracy of these models will decrease if they are used to predict SWCCs of soils having different properties from those in the dataset used in model calibration. The second approach is called the domain method (Braddock et al., 2001; Mualem, 1974; Yao & Vanapalli, 2022), and it is assumed that water in soils is stored in spherical pores with different radii. Each pore only has two states, namely water-filled or empty, and a large pore
corresponds to a low suction. At a given matric suction, there is one equivalent pore radius, and
the corresponding water content in soils is the volume sum of pores whose radius is less than the
equivalent pore radius. Due to the ‘ink-bottle’ effect, during the wetting process, large pores
obstruct the water soaking process, and only part of pores with radius less than the equivalent pore
radius are filled with water (Mualem, 1974; Pham, 2001; Zhai et al., 2020). Therefore, at a given
suction, the water content for the drying process is larger than that for the wetting process, and the
hysteresis of SWCC can thus be captured. However, the domain method cannot show the water
distribution in unsaturated soils well. Apart from liquid moisture transfer, vapor transfer also
contributes to the moisture migration in soils (Chen, 2012). Because of thermal gradients, water
vapor migrates from the high-temperature area to the low-temperature area to equalize the thermal
energy of the two area. Once vapor reaches the cool area, condensation happens. Therefore, the
existence of water is independent of the pore size, and it has been observed experimentally that
due to adsorption and capillary contributions, water accumulates on the grain surface and around
the contact points of grains (Lourenço et al., 2012). The theoretical approach is the most promising
to predict the SWCC of soils, and it has gained increasing attention (Guo et al., 2019; Wang & Li,
2015; Zhang et al., 2013). For example, Beckett & Augarde (2013) used a unit cell with hexagonal
close-packed structure to describe the microstructure of soils, and the pores in the unit cell were
assumed to be spherical. An equation was first used to determine the equivalent pore radius based
on a given matric suction, and then the corresponding water content is the volume sum of pores
with radius less than the equivalent pore radius, the water bridges and water films in unit cells with
pore radius larger than the equivalent pore radius. The thickness of water films was obtained by
considering the effect of van der Waals forces. Since drying processes and wetting processes
follow different relationships between equivalent pore radius and suction, the SWCC hysteresis
could be reflected. Alves et al. (2020) used a unit cell with simple cubic structure to describe the
soil microstructure. Similar to the last model mentioned, each unit cell was composed of spherical
grains with the same radius, and water accumulates around contact points among grains, but water
films on grain surfaces were not considered. To consider the grain size distribution, the soil was
divided into many fractions based on the grain size. For each fraction, the corresponding SWCC
can be obtained based on its unit cell. The SWCC of the soil is the sum of SWCCs corresponding
to these grain size fractions. Fu et al. (2021) proposed an equivalent liquid bridge model to predict
SWCCs of soils. The volume of the liquid bridge between two spheres could be derived from the
water content in soils using a proposed expression. Then, based on the Young-Laplace equation, the suction could be obtained. To consider the grain size distribution, the diameter of these two spheres equals the mean size of the soil, which is defined as the sum of the product of percentage content and minimum size limit of clay, silt, sand and gravel in the soil. By considering the contact angle hysteresis, the SWCC hysteresis was capture.

However, there are still some problems needed to be solved about existing theoretical models on the prediction of SWCC. Firstly, the proposed model should be comprehensive and good for practical application. Most existing models contain empirical parameters, so they are good at fitting, instead of predicting the SWCC. For a good predictive model, every parameter should have clearing physical meaning and their values can be determined based on some easy-to-measure soil properties. For example, Tokunaga (2011) considered the effect of van der Waals forces and electric double-layer forces on the water film thickness in soils, so the model is comprehensive. However, in the model, the water film thickness is expressed as a function of matric potential, which is not easy to measure, and this is not good for the practical application. Secondly, the existing equations used to calculate the volume of liquid bridge between two spheres are questionable. In the three theoretical models mentioned above, three different equations are used to calculate the volume of liquid bridge. This means that there is still no volume calculation equation that can be accepted by most researchers. Thirdly, the mean grain size and the sum of SWCCs corresponding to every grain-size fraction do not perform good on the consideration of the effect of grain-size distribution. The size of gravel is over 1000 times larger than that of clays. If the concept of mean grain size is used, the effect of fine grains may be neglected. Similarly, experiments (Raghuram et al., 2020) show that suction corresponding to fine grains is over 1000 times larger than that corresponding to coarse grains. Thus, if the SWCC of soils is the sum of SWCCs corresponding to every grain-size fraction, the effect of coarse grains will be neglected. Last but not least, the existing models cannot show some new findings. Studies have shown that engineering behavior of soils can be better interpreted if the influence of matric suction is considered (Banerjee et al., 2018; Puppala et al., 2019; Wray et al., 2005), so a good SWCC model should be able to explain some phenomena in soils. For example, it is believed that the swelling of expansive soils is due to the presence of some clay minerals, like Kaolinite, Illite and Montmorillonite (Asuri & Keshavamurthy, 2016; Zhou et al., 2022). The swelling of these clay
minerals in water arises from the repulsive pressure caused by electric double-layer forces (Das & Das, 2008). However, it is still uncertain about the shrinkage mechanism of expansive soils at a low water content (Chen, 2012). If the volumetric change of expansive soils were really controlled by clay minerals, shrinkage should not happen.

In this work, to solve the problems mentioned above, a micromechanics model is proposed to predict the SWCC of unsaturated soils. In the model, every parameter has clear physical meaning and can be determined experimentally. This study is organized as follows. In the next section, a chemical model is proposed to determine the water film thickness in soils and the effects of van der Waals forces and electric double-layer forces are considered. Then, expressions for the volume calculation of the water bridge between two contacted spherical grains are derived, and the SWCC can be obtained by incorporating the liquid bridge model to the representative volume element (RVE) of soils. The contact angle hysteresis is considered to capture the SWCC hysteresis, and the concept of equivalent grain radius is proposed to consider the effect of grain-size distribution. The change of SWCC with the RVE structure is analyzed to illustrate the behavior of soils under wetting-drying cycles. In the result part, several groups of test data are adopted to verify the validity of the proposed models. By analyzing the model predictions, new mechanisms about the swelling and shrinkage of expansive soils are found. The last section summarizes the main findings.
2. Model formulation

2.1. Water film thickness on the surface of solids

![Diagram of the stable water film on the flat surface of solids](image)

**Figure 1.** Diagram of the stable water film on the flat surface of solids

The stability of water film on a solid surface is affected by van der Waals forces and electric double-layer forces (Israelachvili, 2011). In this section, by analyzing the effect of these two types of forces, a new chemical model is proposed to predict the thickness of water film. For practical applications, the film thickness is expressed as a function of some easy-to-measure parameters, like the temperature, relative humidity, and solid geometry in soils.

2.1.1. Effect of van der Waals forces

The van der Waals force between two materials can be attractive or repulsive, and it depends on the dielectric properties of materials. Materials having similar properties in a medium always suffers attractive van der Waals forces, while dissimilar materials in a medium could be attractive
or repulsive. For example, if the dielectric constant of the medium is intermediate between those of the two materials, these two materials will be repelled from each other. The van der Waals force per unit area on the air-water interface, as shown in Figure 1, can be expressed as:

\[ P_{VDW} = -A_{132} / 6\pi d^3 \]  

with

\[ A_{132} = \frac{3}{4} k_B T \left( \frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_1 + \varepsilon_3} \right) \left( \frac{\varepsilon_2 - \varepsilon_3}{\varepsilon_2 + \varepsilon_3} \right) + \frac{3h\nu_e}{8\sqrt{2}} \frac{(n_1^2 - n_3^2)(n_2^2 - n_3^2)}{\left( (n_1^2 + n_3^2)(n_2^2 + n_3^2) \right)^{3/2}} \]  

\[ (\varepsilon_1 + \varepsilon_3)(\varepsilon_2 + \varepsilon_3) \]

where \( A_{132} \) is the nonretarded Hamaker constant for media 1 (solid) and 2 (air) interacting across medium 3 (water), \( d \) the thickness of the water film, \( \nu_e \) the main electronic absorption frequency in the UV, \( k_B \) the Boltzmann constant, \( T \) the temperature in Kelvin, \( n_i \) and \( \varepsilon_i \) (\( i = 1, 2, 3 \)) are the refractive index in the visible and the dielectric constant respectively of phase \( i \). Equation 2 works only when the absorption frequencies for the three phases are the same. Here, it is defined that the sign of pressure is positive.

In some cases, combining relations are often used to approximate the Hamaker constant as below:

\[ A_{i32} = \sqrt{A_i} - \sqrt{A_3} \]  

\[ \approx \sqrt{A_2} - \sqrt{A_3} \]

where \( A_{i3} \) is the Hamaker constant for two media \( i \) interacting across a vacuum. However, combining relations works only when the van der Waal forces dominate the interaction, and they break down when media with high dielectric constants, such as water, are involved. Therefore, Equation 3 cannot be used to determine the thickness of the water film as shown in Figure 1.

From Equation 1, it can be seen that the Hamaker constant is the key to the determination of van der Waals forces. Table 1 summarized the values of Hamaker constants for some materials interacting with air across water, and all the materials have negative values for \( A_{132} \). This means the force between the materials and air is repulsive, and this is good for the stability of water film. From Table 1, it can be concluded the Hamaker constant in soils may be in the order of \( 10^{-20} \text{ J} \).

<table>
<thead>
<tr>
<th>Medium 1</th>
<th>Medium 3</th>
<th>Medium 2</th>
<th>Hamaker constant ( A_{132} ) ( \times 10^{-20} ) J</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fused silica (Hough &amp; White, 1980)</td>
<td>Water</td>
<td>Air</td>
<td>-1.03</td>
</tr>
<tr>
<td>Material</td>
<td>Phase Water</td>
<td>Phase Air</td>
<td>Pressure</td>
</tr>
<tr>
<td>--------------------------------</td>
<td>-------------</td>
<td>------------</td>
<td>----------</td>
</tr>
<tr>
<td>Calcite (Hough &amp; White, 1980)</td>
<td>Water</td>
<td>Air</td>
<td>-2.26</td>
</tr>
<tr>
<td>Calcium fluoride (Hough &amp; White, 1980)</td>
<td>Water</td>
<td>Air</td>
<td>-1.23</td>
</tr>
<tr>
<td>Soils (Or &amp; Tuller, 1999)</td>
<td>Water</td>
<td>Air</td>
<td>-6</td>
</tr>
</tbody>
</table>

Note: $A_{132}$ for soils was determined by fitting adsorption data and the effect of the electric double-layer force was not considered.

2.1.2. Effect of electric double-layer forces

Different from van der Waals forces, electric double-layer forces in a medium are always repulsive. The surface of some solids in water is charged, because of the dissociation of some surface groups. For example, the surface of some clay minerals in water can dissociate and give off $Na^+$, $K^+$, and $Ca^{2+}$ ions. These cations are called counterions and the anions on the surface are called co-ions (here, we do not consider the effect of the $H_3O^+$ and $OH^-$ from dissociated water). Electric double-layer forces arise from the osmotic pressure between the counterions, and they force the counterions away from the solid-water interface and from each other.

Based on the Langmuir equation (Langmuir, 1918), the disjoining pressure arising from electric double-layer forces in the water film can be expressed as:

$$P_{el} = \frac{e^2}{\varepsilon_0 \varepsilon} \left( \frac{\pi k_B T}{z e} \right)^2 / 2d^2$$

(4)

where $e$ is the electron charge, $z$ the ion valence, $\varepsilon_0 (= 8.854 \times 10^{-12} \text{ C}^2 \text{ J}^{-1} \text{ m}^{-1})$ the permittivity of free space, and $\varepsilon (=78.2$ at 25ºC) the dielectric constant of water.

Therefore, based on the additivity assumption, relative to the atmospheric pressure (1 bar), the pressure imposed on the air-water interface from the solid surface is:

$$P_1 = P_{el} + P_{VDW}$$

(5)

If the surface is flat, the relative pressure can be expressed as a function of relative vapor pressure as below (Thomson, 1872):

$$P_2 = -(RT / \nu) \ln(p_v / p_{sat})$$

(6)
where \( R (= 8.314 \text{ J} \cdot (\text{mol} \cdot \text{K})^{-1}) \) is the Avogadro constant, \( v \) the molar volume of water, and \( p_v \) and \( p_{sat} \) are the vapor pressure in the air and the saturated water vapor pressure. Therefore, it can be seen that the water film thickness increases with the relative vapor pressure.

However, for grains in soils, they are assumed to be spherical instead of flat in this work. To account for the effect of grain curvature, the relative pressure is expressed as:

\[
P_z = -(RT / v) \ln(p_v / p_{eq})
\]

where \( p_{eq} \) is the equilibrium vapor pressure.

Since according to the Kelvin equation (Thomson, 1872), the relationship between the equilibrium vapor pressure of a liquid and its saturated vapor pressure can be expressed as:

\[
p_{eq} = p_{sat} \cdot \exp\left(\frac{2\gamma \kappa}{RT}\right)
\]

where \( \gamma \) is the surface energy density or surface tension of water in air, and \( \kappa \) is the mean curvature of water film and it may be approximated using the curvature of the solid surface.

By substituting Equation 8 into Equation 7 and based on the force balance, we can obtain:

\[
P_z = P_z = -(RT / v) \ln(p_v / p_{sat}) + \gamma \kappa = -(RT / v) \ln(RH) + \gamma \kappa
\]

where \( RH (=p_v / p_{sat}) \) is the relative humidity. Combing Equations 5 and 9, the water film thickness can be determined, once the Hamaker constant \((A_{132})\), the ion valence of counterions \((z)\), temperature \((T)\), surface tension of water in air \((\gamma)\), relative humidity in soils \((RH)\), dielectric constant \((\varepsilon)\) and molar volume \((v)\) of water, and the solid surface curvature \((\kappa)\) are known. Here, it is defined that the curvature for convex surfaces is positive, while that for concave surfaces is negative.

However, for soils, they contain different minerals, and different minerals have different chemical compositions and different Hamaker constants. This makes the determination of \( A_{132} \) and \( z \) complicated. To solve this problem, in this work it is assumed that \( z \) equals 1. To determine the value of \( A_{132} \), adsorption data from several groups of soils are used and the constant can be obtained by fitting the test data, as shown in the result part.
2.2. Liquid bridge model for two contacted spheres

With the increase of relative humidity from 0, the water film forms on the surface of solids. Then, since the water meniscus around the contact point of two grains is concave ($\kappa < 0$), as shown in Figure 2(a), based on Equation 8, $p_{eq} < p_{sat}$. Thus, in the vicinity of the concave water meniscus, water vapors in air can reach an over-saturated state easily, and this is good for condensation. Water droplets may form on the surface of grains under dynamic environmental conditions. However, when the system approaches to equilibrium, these water droplets will disappear. That is because these droplets have large curvatures, and this can result in a very high $p_{eq}$, so they can evaporate easily. Therefore, at equilibrium conditions, with the increase of water content in soils, water accumulates around the contact points of grains.
Figure 2. The water distribution around two contacted spherical grains when (a) $\theta + \beta \leq 90^\circ$, and (b) $\theta + \beta > 90^\circ$.

When the water meniscus is concave, as shown in Figure 2(a), based on the Young-Laplace equation (Young, 1805), the capillary pressure or matric suction between these two particles is as below:

$$\psi = u_a - u_w = \gamma \left( \frac{1}{k} - \frac{1}{l} \right)$$

where $u_a$ and $u_w$ are the atmospheric and water pressures respectively, $\gamma$ the air-water surface energy density, $k (\geq 0)$ and $l (\geq 0)$ the meniscus radii of curvature.

Based on the shell method, the water volume between two contacted grains can be calculated as below:
\[
\nu_w = 2\int_0^{\sin \beta} 2\pi x \cdot (r - \sqrt{r^2 - x^2}) \, dx - 2\int_{\sin \beta}^{\pi} 2\pi x \cdot \sqrt{k^2 - [x - (l + k)]^2} \, dx
\]
\[
= 2\pi r^3 \sin^2 \beta + \frac{4\pi r^3}{3}(\cos^3 \beta - 1) + \frac{4\pi}{3}[k^2 - (r \sin \beta - l - k)^2]^{3/2}
+ \pi(l + k)[2(r \sin \beta - l - k)\sqrt{k^2 - (r \sin \beta - l - k)^2} + \pi k^2
+ 2k^2 \arcsin(\frac{r \sin \beta - l - k}{k})]
\]

(11)

with

\[
k = \frac{r(1 - \cos \beta)}{\cos(\theta + \beta)}
\]

(12)

\[
l = r \sin \beta - k + k \sin(\theta + \beta)
\]

(13)

\[
r = r_0 + d
\]

(14)

where \(\nu_w\) is the volume of water around the contact point, \(\theta\) the contact angle, \(r_0\) the radius of the spherical grains, \(d\) the thickness of the water film and \(\beta\) the angle related to the volumetric water content. Since from the result part it can be seen that the water film thickness is very small compared to the radius of grains even at high relative humidity, it is rational to approximate \(r\) using the sum of the grain radius and water film thickness.

From Equations 10-14, it can be seen that once \(\nu_w, \theta\) and \(r\) are known, the suction can be determined and the value of \(\beta\) can be obtained based on Equation 11. From Equation 12, it can be found that the formula only applies to the condition when \((\theta + \beta)\) is less than 90º. Otherwise, \(k\) is negative and it is conflict with Equation 10. For hydrophilic materials, even though \(\theta\) is less than 90º, with the increase of volumetric water content, \(\beta\) increases. Thus, the condition when \((\theta + \beta) > 0\) exists and it has been observed experimentally (Lourenço et al., 2012).

When the water meniscus is convex, as shown in Figure 2(b), \((\theta + \beta) > 90^\circ\) and the capillary pressure or matric suction between these two particles is as below:

\[
\psi = u_a - u_w = -\gamma(\frac{1}{k} + \frac{1}{l})
\]

(15)
The volume of water around the contact point can be calculated as below:

\[
v_w = 2\int_0^{r\sin\beta} 2\pi x \cdot (r - \sqrt{r^2 - x^2}) dx + 2\int_{r\sin\beta}^l 2\pi x \cdot \sqrt{k^2 - [x - (l - k)]^2} dx
\]

\[
= 2\pi r^3 \sin^2 \beta + \frac{4\pi r^3}{3} (\cos^3 \beta - 1) + \frac{4\pi}{3} [k^2 - (r\sin \beta - l + k)^2]^{3/2}
\]

\[
+ \pi (l + k) [\pi k^2 - 2(r\sin \beta - l + k)\sqrt{k^2 - (r\sin \beta - l + k)^2}
\]

\[-2k^2 \arcsin\left(\frac{r\sin \beta - l + k}{k}\right)]
\]

with

\[
k = \frac{r(1 - \cos \beta)}{\cos(\theta + \beta)} \quad (17)
\]

\[
l = r\sin \beta + k - k\sin(\theta + \beta) \quad (18)
\]

Similarly, when the water meniscus is convex, based on Equations 15-18, once \(v_w, \theta \) and \(r \) are known, the suction can be determined and its value is negative. The value of \(\beta \) can be determined using Equation 16. Arising from the chemistry and topography of solid surfaces, the advancing contact angle \((\theta_a)\) and receding contact angle \((\theta_r)\) of liquid on solid surfaces are different, and \(\theta_a\) is usually larger than \(\theta_r\). Therefore, to consider the contact angle hysteresis, when it is wetting, \(\theta_a\) is used to replace \(\theta\) in the formula above. When it is drying, \(\theta_r\) is used to replace \(\theta\) in the formula.

2.3. Microstructure of soils

If the soil is composed of grains with only one size, the soil microstructure can be represented using one type of representative volume element (RVE). The RVE structure can be described using the body-centered cubic (BCC) structure, face-centered cubic (FCC) structure, hexagonal close-packed (HCP) structure or simple cubic (SC) structure, as shown in Figure 3.
For the BCC structure, as shown in Figure 3(a), grains are located at corner and center position. The volume of the RVE is:

$$V = \frac{64r_0^3}{3\sqrt{3}}$$

where $r_0$ is the radius of the grain.

**Figure 3.** Representative volume element structure of soils.
The total number of grains in the RVE is:

\[ N = 2 \]  

(20)

Porosity \( n \) is defined as the ratio of the volume of voids to the total volume in the RVE, so the porosity of BCC is as below:

\[ n = 0.32 \]  

(21)

The total number of complete contact points is:

\[ M = 8 \]  

(22)

Therefore, once the volumetric water content (VWC) in soils is known, the water volume around each contact point (\( \nu_w \)) can be obtained as below. In this work we assume \( \nu_w \) in each complete contact point is equal.

\[ \nu_w = \frac{VWC \cdot V - V_{w0}}{M} \]  

(23)

with

\[ V_{w0} = \frac{4N}{3} \pi [(r_0 + d)^3 - r_0^3] \]  

(24)

where \( V_{w0} \) is the volume of water films on the grain surface in the RVE, and it corresponds to the residual volumetric water content.

Thus, once the microstructure of the soil and the contact angles (including advancing angle and receding angle) are known, based on Equations 10-18, the relationship between \( \nu_w \) and \( \psi \) can be determined.

The properties for different RVE structures are summarized in Table 2. It can be seen that SC structure has the largest porosity, while FCC and HCP structures have the lowest porosity. It needs to be noted that the above mentioned four types of RVE structure are approximations to the real structure of soils and the most accurate way to determine the RVE of soils is by doing experiments. The microstructure of soils can be described based on the volume, porosity, grain size and number of complete contact points in the RVE.
Table 2: Properties of representative volume elements of soils

<table>
<thead>
<tr>
<th>Microstructure</th>
<th>BCC</th>
<th>FCC</th>
<th>SC</th>
<th>HCP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume ((V))</td>
<td>(64r_0^3/3\sqrt{3})</td>
<td>(16\sqrt{2}r_0^3)</td>
<td>(8r_0^3)</td>
<td>(24\sqrt{2}r_0^3)</td>
</tr>
<tr>
<td>Number of grains ((N))</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>6</td>
</tr>
<tr>
<td>Porosity ((n))</td>
<td>0.32</td>
<td>0.26</td>
<td>0.48</td>
<td>0.26</td>
</tr>
<tr>
<td>Number of complete contact points ((M))</td>
<td>8</td>
<td>24</td>
<td>3</td>
<td>27</td>
</tr>
</tbody>
</table>

Note: BCC: Body-centered cubic; FCC: Face-centered cubic; SC: Simple cubic; HCP: Hexagonal close-packed; \(r_0\): Radius of the grain.

2.3.1. Effect of grain-size distribution

A naturally occurring soil sample usually has grains of various size, and based on the size of grains, soils can be divided into gravel, sand, silt and clay. According to the classification of the U.S. department of agriculture, the size of gravels is larger than \(2\ \text{mm}\); the size of sands is from \(0.05\ \text{mm}\) to \(2\ \text{mm}\); the size of silt is from \(0.002\ \text{mm}\) to \(0.05\ \text{mm}\); the size of clay is less than \(0.002\ \text{mm}\). The grain-size distribution of coarse-grained soils is determined by sieve analysis, and these grains are larger than \(0.075\ \text{mm}\). For fine-grained soils, hydrometer analysis is used for determination of the grain-size distribution, and it is based on the principle of sedimentation of soil grains.

To consider the grain-size distribution, a concept of equivalent grain radius is proposed as below:

\[
 r_{\text{eq}} = \frac{10^{x_{\text{eq}}}}{2} \tag{25}
\]

with

\[
 x_{\text{eq}} = \sum_i c_i \cdot \log_{10}(L_i) \tag{26}
\]

where \(r_{\text{eq}}\) is the equivalent grain radius in soils, \(L_i\) is the size of the \(i\)th sieve, and \(c_i\) is the percentage of soils retained on the \(i\)th sieve. Standardization can be realized by taking the logarithm to the grain or sieve sizes, and by taking the average of standardized sizes, the effect of very small grains can be considered.

If a soil contains several types of RVE, the matric suction of the soil can be expressed as:
\[ \Psi = \sum_{j=1}^{4} p_j \psi_j \left( r_{eq} \right) \]  
\[(27)\]

where \( j \) represents the type of RVE structure, and 1, 2, 3, 4 represent BCC, FCC, SC, HCP respectively; \( p_j \) represents the percentage of RVE structure type \( j \) in the soil and \( \sum_{j=1}^{4} p_j = 1; \psi_j \) represents the matric suction in a RVE with structure type \( j \).

2.3.2. Evolution of the RVE structure

![Figure 4. Separation of two contacted grains because of the negative matric suction.](image)

As will be seen in the result, for fine-grained soils, when they approach to be saturated, the matric suction is negative and the pressure difference can force contacted particles separated. Figure 4 shows the separation of two contacted particles. Water pressure pushes two particles outwards, while surface energy pulls these two particles inwards. Therefore, the net force between two contacted grains is as below:

\[ F = (u_w - u_a) \cdot \pi (r \sin \beta)^2 - 2\pi r \sin \beta \cdot \gamma \cos(\theta + \beta - \frac{\pi}{2}) \]
\[= \pi r \sin \beta \cdot [(u_w - u_a) r \sin \beta - 2\gamma \cdot \sin(\theta + \beta)] \]  
\[(28)\]

Therefore, if we do not consider forces from the surrounding, when \( F > 0 \), these two grains start to separate. Separation may also happen between two contacted grains with a concave water meniscus. As shown in Equation 10, when \( k > l \), the matric suction is negative, so the separation criterion can be obtained based on the procedure above.
Although during drying, high positive matric suction will bind particles together, the chaos increases with the increase of the wetting-drying cycle number, based on the second law of thermodynamics. It has been observed experimentally that wetting-drying cycles can increase the porosity of soils (Pires et al., 2005; Pires et al., 2009). Therefore, every wetting-drying cycle can be regarded as a process of rearrangement of grains, and the RVE structure of soils may be different in different wetting-drying cycles. This can explain the change of the soil water characteristic curve after wetting-drying cycles.

3. Results

3.1. Water film thickness

To determine the value of Hamaker constant \( A_{132} \) of soils and verify the validity of the water film thickness model proposed, some test data (Campbell & Shiozawa, 1992; Or & Hanks, 1992) are adopted. These data were collected by Or and Tuller (Or & Tuller, 1999), and they obtained the value of \( A_{132} \) by fitting the data using a film adsorption equation they proposed. They found the water film thickness in soils with mixed clay minerals could be described by a single \( A_{132} \). However, in their model, the effect of electric double-layer forces on the water film thickness is not considered. In this part, we follow the same procedure as that of Or and Tuller to determine the value of \( A_{132} \) in the proposed model by fitting test data. As shown in Table 3, the data set is composed of six groups of soils, so the data set is representative in terms of grain-size distribution and soil textures.

<table>
<thead>
<tr>
<th>Soil series</th>
<th>Sand</th>
<th>Silt</th>
<th>Clay</th>
<th>Clay minerals</th>
<th>Porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>L-Soil (Campbell &amp; Shiozawa, 1992)</td>
<td>0.888</td>
<td>0.061</td>
<td>0.051</td>
<td>Mixed</td>
<td>0.45</td>
</tr>
<tr>
<td>Royal (Campbell &amp; Shiozawa, 1992)</td>
<td>0.536</td>
<td>0.319</td>
<td>0.145</td>
<td>Mixed</td>
<td>0.48</td>
</tr>
<tr>
<td>Walla Walla (Campbell &amp; Shiozawa, 1992)</td>
<td>0.228</td>
<td>0.633</td>
<td>0.139</td>
<td>Mixed</td>
<td>0.52</td>
</tr>
<tr>
<td>Millville (Or &amp; Hanks, 1992)</td>
<td>0.330</td>
<td>0.490</td>
<td>0.180</td>
<td>Mixed</td>
<td>0.47</td>
</tr>
</tbody>
</table>
Table 4 Values of parameters used in the model prediction.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Saturated vapor pressure ($p_{sat}$)</td>
<td>3169 Pa</td>
<td>Water surface tension ($\gamma$)</td>
<td>72 mN/m</td>
</tr>
<tr>
<td>Hamaker constant ($A_{132}$)</td>
<td>$-3.5 \times 10^{-20}$ J</td>
<td>dielectric constant ($\varepsilon$)</td>
<td>78.2</td>
</tr>
<tr>
<td>Ion valence ($z$)</td>
<td>1</td>
<td>water molar volume ($v$)</td>
<td>18.07 cm$^3$/mol</td>
</tr>
<tr>
<td>Temperature ($T$)</td>
<td>25°C</td>
<td>Radius of spherical solids ($r_0$)</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Figure 5 shows the comparison between test data and model predictions on the water film thickness, and values of parameters used during model prediction are summarized in Table 4. It can be seen that when $A_{132}$ equals $-3.5 \times 10^{-20}$ J, the model prediction matches the test data well, and a single $A_{132}$ is able to describe the change of the water film thickness with vapor pressure in soils. The value of $A_{132}$ obtained is less than the value ($A_{132}=-6\times10^{-20}$ J) obtained by Or and Tuller (Or & Tuller, 1999). That is because we considered the effect of both van der Waals forces and electric double-layer forces. In the model prediction, it is assumed that soils are composed of spherical grains with radii equal 1 mm. To verify the effect of grain size on the water film thickness, parameter analysis is done, as shown in Figure 6. It can be seen that when the relative humidity ($RH$) is less than 0.99, the effect of grain size on the water film thickness is negligible. This may explain why a single $A_{132}$ applies to soils with different gradations. From Figure 6(b), it can be seen that when $RH$ is higher than 0.99, the effect of grain size on the film thickness increases and cannot be neglected. The water film thickness also increases with the increase of the grain size.
Figure 5. Comparison between test data (Or & Tuller, 1999) and model prediction on the change of water film thickness with water vapor pressure in soils.

Figure 6. Effect of grain size on the water film thickness.

3.2. SWCC

To verify the validity of the proposed model on the prediction of SWCC, test data from a literature (Zhang & Li, 2010) is adopted. In the literature, the relationships between gravimetric water content and matric suction of five types of soils were measured, and the gradations for the soils are shown in Figure 7. These soils were classified as CL (lean clay with sand), ML (sandy silt),
SC (clayey sand with gravel), SM (silt sand with gravel), and GW-GM (well-graded gravel with silt and sand) based on ASTM D2487 (ASTM, 2011). In this work, the measured relationship between gravimetric water content and matric suction is converted to that between volumetric water content and matric suction using the equation below:

\[ w = \frac{VWC \cdot \rho_w}{\rho_d} \]  

(29)

where \( VWC \) is the volumetric water content, \( w \) the gravimetric water content, \( \rho_w \) the density of water and \( \rho_d \) the dry density of soil. The test data about \( \rho_d \) of these five types of soils are summarized in Table 5.

It is assumed the relative humidity of these soils is 99%, and the temperature is 25°C. The equivalent grain radius can be obtained based on their gradation using Equation 25. Since the RVE structures and contact angles of these soils were not analyzed, it is assumed that these five types of soils have the same microstructure, but have different contact angles. The soil properties are summarized in Table 5, and comparison between model predictions and test data is shown in Figure 8. Although the good match between model predictions and test data is achieved by adjusting the contact angle and accuracy of model prediction is not verified due to the lack of information about the microstructure and contact angle of soils, it shows that the proposed model has the ability to capture the SWCC of soils.
Figure 7. Gradation of five types of soils (Zhang & Li, 2010).

Table 5 Soil properties.

<table>
<thead>
<tr>
<th>Soil name</th>
<th>Dry density (Zhang &amp; Li, 2010) (kg/m³)</th>
<th>Equivalent grain radius $r_{eq}$ (mm)</th>
<th>Contact angle (°)</th>
<th>RVE volume $V$ (cm³)</th>
<th>RVE porosity</th>
<th>Complete contact points number in RVE</th>
</tr>
</thead>
<tbody>
<tr>
<td>CL</td>
<td>1550</td>
<td>0.0108</td>
<td>10</td>
<td>0.0101</td>
<td>0.6</td>
<td>13</td>
</tr>
<tr>
<td>ML</td>
<td>1710</td>
<td>0.0365</td>
<td>26</td>
<td>0.389</td>
<td>0.6</td>
<td>13</td>
</tr>
<tr>
<td>SC</td>
<td>1900</td>
<td>0.1204</td>
<td>28</td>
<td>14.0</td>
<td>0.6</td>
<td>13</td>
</tr>
<tr>
<td>SM</td>
<td>1970</td>
<td>0.3939</td>
<td>28</td>
<td>488.9</td>
<td>0.6</td>
<td>13</td>
</tr>
<tr>
<td>GW-GM</td>
<td>1950</td>
<td>1.3185</td>
<td>41</td>
<td>18337.1</td>
<td>0.6</td>
<td>13</td>
</tr>
</tbody>
</table>

Note: $V = 8r_{eq}^3$. 
Figure 8. Comparison between test data (Zhang & Li, 2010) and model predictions.
The effect of equivalent grain radius, contact angle and microstructure of soils on the SWCC are studied by doing parametric analysis. Figure 9 shows SWCCs of soils with different grain sizes and contact angles. By comparing curves \((r_{eq} = 2\, \mu m, \theta = 10^\circ)\) and \((r_{eq} = 2\, \mu m, \theta = 30^\circ)\), or curves \((r_{eq} = 500\, \mu m, \theta = 10^\circ)\) and \((r_{eq} = 500\, \mu m, \theta = 30^\circ)\), it can be seen that a large contact angle can lead to a low suction. The curve with a low \(\theta\) can represent the drying curve, while the curve with a large \(\theta\) can represent the wetting curve. At a given water content, the suction corresponding to the drying curve is larger than the wetting curves. It shows that the proposed model can capture the SWCC hysteresis. It can also be seen that with the increase of the grain size, the matric suction decreases. This coincides with experimental observations. For example, suction can pull water up a larger distance in a small-radius tube than that in a large-radius tube.

**Figure 9.** Soil-water characteristic curves for soils with BCC structure and \(\gamma\) equal 72mN/m.
Figure 10. Soil-water characteristic curves for soils with BCC structure and γ equal 72mN/m when the soils approach to be saturated. (a) $r_{eq}=2\mu$m; (b) $r_{eq}=500\mu$m.

Since in Figure 9, the scale of the abscissa is in logarithm, only predictions with positive suction values can be plotted. Figure 10 shows the change of matric suction when the soil approaches to be saturated. A negative matric suction means the pressure within the water meniscus ($u_w$) is larger than the atmospheric pressure ($u_a$), and if the pressure difference is large enough, two contacted grains can be separated. By comparing Figures 10(a) and 10(b), it can be found that when the soil approaches to be saturated, ($u_w - u_a$) decreases with the increase of the grain size or with the decrease of the contact angle. This can explain the swelling and shrinking mechanisms of expansive soils. Expansive soils contain incredibly fine particles. When they approach to be saturated, extremely large pressure difference ($u_w - u_a$) forces contacted grains separated, which can lead to swelling. When they are drying out, the matric suction is extremely large, as shown in Figure 9, so it causes the shrinkage. Such large suction also explains why it is difficult to drain expansive soils.
Figure 11. Soil-water characteristic curves for soils with different RVE structure and contact angles ($r_{eq} = 1 \text{mm}$ and $\gamma = 72 \text{mN/m}$).

Figure 11 shows SWCCs for soils with different RVE and contact angles. By comparing the results for FCC, BBC and SC, it can be found that with the increase of the porosity, the predicted SWCC moves downwards. This has been verified by many phenomena that a high porosity can cause a low suction. For example, because of the suction, the water from underground can move to the ground surface, and to prevent the loss of water, farmers usually loose soils to prevent the evaporation by increasing the soil porosity. Since wetting-drying cycles can increase the porosity of soils, this means the proposed model is capable of capturing the suction decrease after wetting-drying cycles by considering the change of soil RVE structure. In addition, experiments (Miller et al., 2008) show that at the same suction, the volumetric water content corresponding to a high normal stress is higher than that corresponding to a low net normal stress. A high net normal stress can cause a low porosity, and from Figure 11, it can be concluded that the proposed model can capture the experimental observation well. By comparing SWCCs for FCC and HCP, it can be seen that although the HCP structure has more complete contact points, the slope for HCP is lower that for FCC. That is because the RVE volume of HCP is larger than that of FCC. When the volumetric water content is the same for both structures, the water volume around every contact point in HCP is larger than that in FCC, and the matric suction between contacted grains decreases with the increases of water volume around the contact point.
4. Summary

A chemical model is first proposed to determine the adsorbed water film thickness on the grain surface by considering the effect of van der Waals forces and electric double-layer forces. The film thickness can be determined through some easy-to-measure variables, like the relative humidity, water surface tension in air and solid surface curvature. Then, a micromechanics model is proposed to predict the SWCC of soils. The expression for water volume and suction between two contacted spherical grains are derived, and by studying the microstructure of soils, the SWCC can be obtained. Main findings are summarized as below:

1. The proposed water film thickness model and SWCC model are practical. Every parameter in the models has clear physical meaning and is measurable easily.
2. The effect of grain size on the water film thickness is negligible when the relative humidity is less than 99%, and the film thickness is in the order of nanometer.
3. The proposed SWCC model can capture the performance of soils well. It is shown that the huge positive and negative matric suction is responsible for the shrinkage and expansion of expansive soils, which contains very small particles.
4. Matric suction increases with the decrease of grain size and contact angle of water in soils.
5. The decrease of matric suction after wetting-drying cycles arises from the change of soil microstructure, and matric suction decreases with the increase of porosity.

In the future, the microstructure of soils and contact angle of water in soils will be further studies.

Acknowledgments

The authors declare no conflicts of interest relevant to this study.

Open Research

Data is available through Or & Tuller, 1999 and Zhang & Li, 2010.
References


