

Article

Effects of Grain Size, Density, and Contact Angle on the Soil–Water Characteristic Curve of Coarse Granular Materials

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Abstract

The soil–water characteristic curve (SWCC) is essential for understanding hydraulic behavior in geotechnical applications involving coarse granular materials. However, existing models often overlook the coupled effects of key factors. This study systematically investigates the influence of grain size distribution, density, and contact angle on the SWCC using a numerical approach that combines the discrete element method (DEM) with an enhanced pore morphology method incorporating locally variable contact angles (Lvca-PMM). The results show that smaller uniformity coefficients (C_u), larger median grain sizes (D_{50}), higher porosity (ϕ), and larger contact angles (θ) shift the SWCC to the left, reducing both the air entry value (Ψ_a) and residual suction (Ψ_r). Specifically, linear relationships were identified between Ψ_a , Ψ_r , C_u , ϕ , and $\cos(\theta)$, while a power-law relationship was observed with D_{50} . Furthermore, the interaction of these factors plays a critical role, where a change in one property can amplify or diminish the effects of others. Based on these findings, empirical equations for predicting Ψ_a and Ψ_r were developed, offering practical tools for engineers to efficiently estimate the SWCC. This research provides deeper insight into the water retention properties of coarse soils and supports the optimized design of granular fills and drainage systems.

Keywords: SWCC; coarse granular materials; grain size distribution; density; contact angle; Lvca-PMM



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1. Introduction

The soil–water characteristic curve (SWCC), also known as the water retention curve, representing the water storage capacity of the soil subjected to its suctions, is defined as the constitutive relationship between suction and the amount of water stored in the soil. The SWCC has been identified as a fundamental tool in unsaturated soil hydromechanics, providing insights into water retention, permeability, and shear strength of soil [1–5]. Therefore, the soil–water retention behavior is important for many applications in geotechnical engineering, such as the design of capillary barrier systems, the assessment of slope stability under unsaturated conditions, and the prediction of moisture movement and evaporation in subgrades [6–8].

Soil–water retention is governed by capillary action, whereby water is held within the soil pores by surface tension. The strength of this capillary force is fundamentally influenced by the contact angle between the water meniscus and the soil particles, which quantifies the soil’s wettability. Consequently, the SWCC is highly nonlinear and strongly dependent on both the pore structure, which is a function of grain size distribution and

density, and the soil–water contact angle. Many scholars have studied the factors affecting the SWCC. For example, in a series of advanced studies, Pasha and Khoshghalb [9–12] developed image-based and DEM-assisted frameworks that link pore morphology and contact angle variability to SWCC behavior. Their work employed both micro-CT imaging and stochastic morphological methods to directly quantify how pore scale features such as pore connectivity, coordination number, and surface roughness influence air entry value (Ψ_a) and residual suction (Ψ_r), providing profound insights into the underlying physical mechanisms. Gallage and Uchimura [13] conducted a series of draining tests to study the effects of grain size distributions and void ratios on SWCC for sandy soils. Their results indicated that the Ψ_a and Ψ_r of sandy soils show linear relationships with grain size and void ratio. However, the effect of void ratio varies with grain size, and, similarly, the influence of grain size is contingent upon the void ratio. This interdependence suggests that the simple linear models are, in fact, a reflection of a more complex synergistic interaction between the two factors. Based on his experimental data, Sakaki [14] subsequently developed power functions to predict the air entry value based on the mean grain size and uniformity coefficient (C_u). Ustohal et al. [15] and Ishakoglu and Baytas [16] experimentally investigated the soil–water characteristic curve (SWCC) of Ottawa sand using liquids with different contact angles and found that the contact angle has a significant impact on the SWCC. However, a critical gap persists in the current understanding. While the individual effects of these parameters have been explored, studies that systematically quantify their coupled and synergistic influences are scarce. Many existing models fail to concurrently incorporate grain size distribution, density, and wettability (contact angle), leading to potential inaccuracies in prediction. Furthermore, there is a lack of quantitative ready-to-use empirical models that encapsulate these interactions for predicting key SWCC parameters.

Measuring SWCC through laboratory experiments is often time-consuming and costly, as are the measurements of contact angle and surface tension. As an alternative, various numerical methods are developed to model the pore scale fluid–fluid flow process. These include (i) models based on lattice or dissipative particle dynamics such as the lattice Boltzmann method [17], (ii) continuum models like volume-of-fluid methods [18], and (iii) morphological methods like the pore morphology method (PMM) models [19–21]. It has been noted that the first two approaches demand substantial computational resources [22,23]. In contrast, pore morphology models (PMMs) are less computationally intensive and can be directly applied to any given microporous structure. PMMs offer a quasi-static representation of the wetting and non-wetting phases in a three-dimensional domain without requiring the solution of the Navier–Stokes equations. Following the foundational work of Hilpert and Miller (2001), PMMs have been extensively used to estimate SWCC for various porous media, including soils [20,21,24], and components of polymer electrolyte fuel cells, such as the gas diffusion layer and microporous layer [25]. By requiring fewer computational resources, PMMs yield results comparable to those obtained from micro- and macro-experimental observations, continuum models, and lattice-based models [20,22,26]. The original PMMs were developed based on an assumption that the fluid maintained a zero contact angle with the solid surfaces. Recently, the authors of [21] introduced the Lvca-PMM approach, which incorporates locally variable contact angles, enabling the simulation of air and water distribution inside porous media under different contact angle scenarios.

The objective of this study is to investigate the joint influence of grain size distribution, density, and contact angle on SWCC by using the Lvca-PMM approach. A series of granular materials with varying grain size distributions and densities are generated by using the discrete element method (DEM). Subsequently, the Lvca-PMM is applied to these porous domains to simulate SWCCs under different contact angle scenarios. The effects of uniformity coefficient (C_u), median grain size (D_{50}), porosity (φ), and contact

angle (θ) on the SWCC behavior, particularly on key SWCC variables, namely air entry values (Ψ_a) and residual suctions (Ψ_r), are investigated. Furthermore, novel empirical functions are developed to estimate Ψ_a and Ψ_r . The primary originality of this work lies in this comprehensive coupled analysis of multiple factors, the application of the advanced Lvca-PMM framework, and the development of these new predictive equations.

2. Methods

2.1. Lvca-PMM Model

The PMM was established by Hilpert and Miller [19] to simulate the quasi-static drainage process in totally wetting (i.e., contact angle $\theta = 0^\circ$) porous media. The physical model is a voxelized medium with one side connected to a non-wetting phase (NWP) reservoir and the opposite side connected to a wetting phase (WP) reservoir. The PMM utilizes two mathematical morphological operations, referred to as erosion and dilation, to reproduce the distributions of WP and NWP inside the porous media with increasing suctions. By using the Minkowski subtraction $\ominus$ and addition $\oplus$, the morphological erosion $\mathcal{E}$ and dilation $\mathcal{D}$ of a binary image A by image B can be expressed as $\mathcal{E}_B(A) = A \ominus B$ and $\mathcal{D}_B(A) = A \oplus B$, respectively. The erosion shrinks the digital pore space, while the dilation expands the remaining pore spaces that are connected to the NWP reservoir. Both erosion and dilation are carried out by using a structuring element, a sphere for three-dimensional simulation. The radius of the sphere is the radius of the curvature of the WP-NWP interface and can be calculated by using the Young–Laplace equation, i.e.,

$$\Psi = 2\gamma/r \quad (1)$$

where γ is the surface tension and Ψ is suction.

For non-zero contact angles scenarios, however, the original PMM is inapplicable. Instead, the authors [21] have developed a Lvca-PMM to simulate the distribution of WP and NWP inside porous media. In the Lvca-PMM, solid phases are dilated by the virtual sphere $B'(D')$ with diameter $D' = 2r'$, i.e., $\mathcal{D}_{B'}(G)$, where G represents solid space. r' is calculated by

$$r' = \sqrt{R^2 + r^2 + 2Rrcos\theta} - R \quad (2)$$

where R is the radius of the particle.

The remaining pore space $P' = [\cup \mathcal{D}_{B'}(G)]^c$ is the complementary subspace of the dilation of solid space. Then, the remaining pore space that is connected to NWP reservoir, $\mathcal{C}(P')$, is dilated by using the virtual sphere $B(D)$ with diameter $D = 2r$, with r calculation by Equation (1). The NWP-filled portion of pore space can be determined by

$$P^n = [\mathcal{C}(P') \oplus B(D) - G] \quad (3)$$

As the straightforward dilation of $\mathcal{C}(P')$ with the virtual sphere of diameter D would hit the solid space G since $D' < D$; hence, G should be subtracted from $\mathcal{C}(P') \oplus S$. The corresponding WP saturation is now calculated by

$$S^w(D) = 1 - \frac{\text{Vol}[\mathcal{C}[\cup \mathcal{D}_{B'}(G)]^c \oplus S(\Phi) - G]}{\text{Vol}[P]} \quad (4)$$

where $\text{Vol}[X]$ represents the volume of X .

Figure 1 shows an example of utilizing the Lvca-PM approach to reproduce the drying SWCC of two unsaturated granular materials. The experimental results of primary drainage tests for glass beads EU-165 and WG were reported in Alves et al. [27]. The grain size distribution is shown in Figure 1a. The drying SWCC for EU-165 and WG was first

measured by desaturated water from the samples (Figure 1b). The measured contact angle between the air–water interface and the glass was 39.8° [28]. Two drainage tests were further performed on EU-165 using Triton X-100 and sodium chloride (NaCl) aqueous solutions that artificially alter surface tension and the contact angle (Figure 1c). For a 0.2 g/L Triton X-100 aqueous solution, Karagunduz et al. [29] measured a surface tension of 3.28×10^{-2} N/m and a contact angle of 12.6° on glass. According to Sghaier et al. [28], a NaCl water solution with a mass concentration of 20% at 20°C exhibits a surface tension of 7.97×10^{-2} N/m and a contact angle with glass of 56.5° on glass. To reproduce the experimental SWCCs, two compressed glass bead samples consisting of 10,000 spherical particles are first generated by using the three-dimensional DEM model [30,31] following the same grain size distributions (see Figure 1a) with the same porosities of 0.354 and 0.334 for EU-165 and WG, respectively [27]. The numerical spherical packing is represented in digital space using voxels with a resolution of $4\ \mu\text{m}$. The Lvca–PMM is then applied to the digital space to reproduce the SWCCs using the same surface tensions and contact angles as in the laboratory tests. Figure 1b,c show the comparisons between the SWCCs modeled by the Lvca–PMM and the experimental results [27]. As shown in Figure 1b,c, the Lvca–PMM model exhibits an excellent predictive capability, successfully reproducing the experimental SWCCs with R^2 values greater than 0.95. It is important to note that the primary objective of this comparison is to validate the Lvca–PMM’s core functionality in simulating drainage under different contact angles, using the well-defined geometry of glass beads as a clear benchmark. The efficacy of the Lvca–PMM approach for modeling fluid distribution in porous media under varied wettability conditions is further supported by its successful application in other studies, such as Bhatta et al. [32] and Gautam et al. [33]. Therefore, this validation confirms the model’s suitability for the subsequent parametric study on coarse granular materials, which is the central focus of this work.

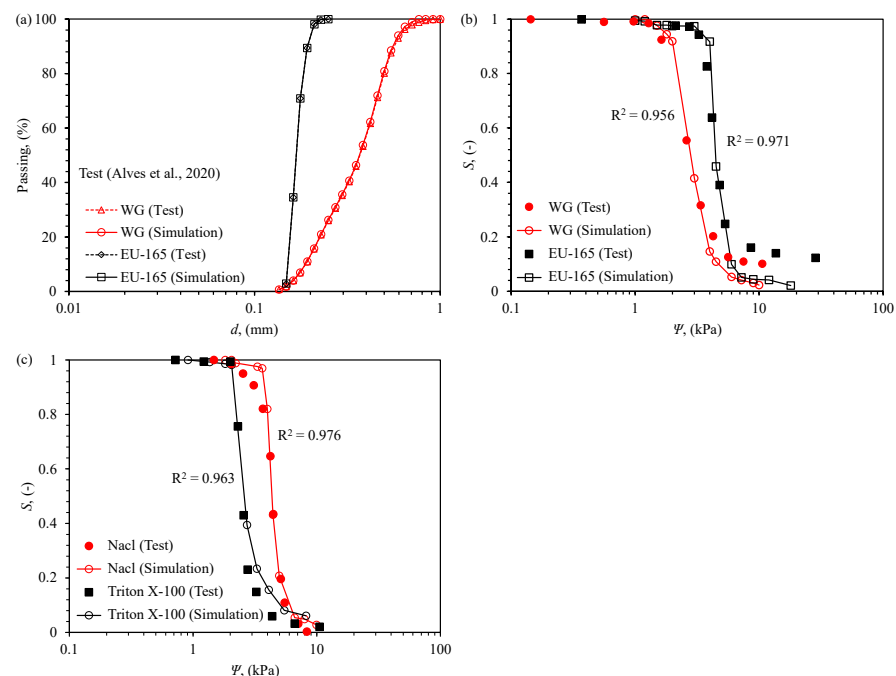


Figure 1. Comparison between the simulated SWCCs and experimental data: (a) grain size distributions; (b) SWCCs of glass bead EU-165 and WG by desaturating water; (c) SWCCs of the glass bead EU-165 by desaturating NaCl and Triton X-100. Experimental data are taken from Alves et al. [27].

2.2. SWCC Variables

The degree of saturation (S), calculated by Equation (4), is fitted by the Fredlund and Xing equation [34],

$$S = \left[1 - \frac{\ln(1 + \Psi/C_r)}{\ln(1 + 10^6/C_r)} \right] \frac{1}{\{\ln[e + (\Psi/a)^n]\}^m} \quad (5)$$

where a , n , and m are fitting parameters; C_r is an input value that can be related to the residual suction. Following Zhai et al. [35], the value of C_r has negligible effects on the performance of Equation (5). Therefore, for simplicity, C_r is assumed to be 1500 kPa in this study after Fredlund and Xing [34], Zhai et al. [35], and Gao et al. [36]. The definition and geometrical relationship of Ψ_a and Ψ_r are illustrated in Figure 2 after Gallage and Uchimura [13] and Zhai et al. [35].

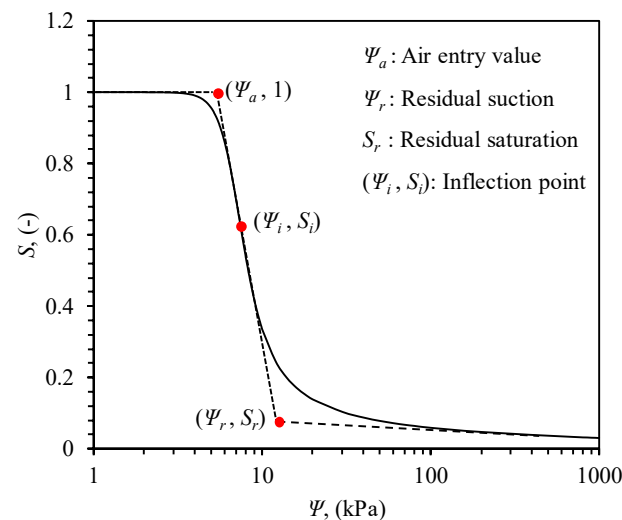


Figure 2. Definitions of SWCC variables (i.e., air entry value and residual suction).

2.3. Numerical Setup

A total of 65 drainage simulations were performed by using Lvca-PMM in this study to investigate the effect of grain size distribution, porosity, and contact angle on the SWCC. At first, three groups of samples, namely, Group A, B, and C, were generated by using the three-dimensional DEM model [30,31] with different C_u , D_{50} , and ϕ . The grain size distributions of samples Group A and B are presented in Figure 3a and Figure 3b, respectively. The grain sizes of the particles range from 0.075 mm to 2 mm, which is in the particle size range of sand as per China standard (GB/T50145 2007) [37]. In Group A, C_u ranges from 1.5 to 4, with D_{50} and ϕ remaining constant. In Group B, D_{50} increases from 0.15 mm to 0.5 mm, while C_u and ϕ remain unchanged. This range of the C_u and D_{50} values falls well within the typical spectrum for pure sand [14]. In Group C, ϕ changes from 0.36 to 0.42, while C_u and D_{50} hold constant. Although the overall range of porosity is relatively narrow due to the limited grain size range adopted in this study, the selected ϕ values are characterized as representing three key density states (loose, medium dense, and dense) based on our DEM simulations. This deliberate variation allows for a systematic investigation into the influence of soil density on the soil–water characteristic curve, while effectively isolating the effects of particle size distribution. Then, Lvca-PMM simulations are conducted by using these samples under a range of contact angles ($\theta = 0^\circ, 20^\circ, 40^\circ, 60^\circ$, and 80°). The θ values were selected to represent a wide range of wettability conditions, from perfectly wetting (0°) to weakly hydrophilic (80°), encompassing both natural soil conditions and scenarios involving contaminated or engineered surfaces. The surface tension is assumed

to be 7.2×10^{-2} N/m, consistent with the surface tension of the air–water interface at 20 °C. The properties of the numerical samples are listed in Table 1.

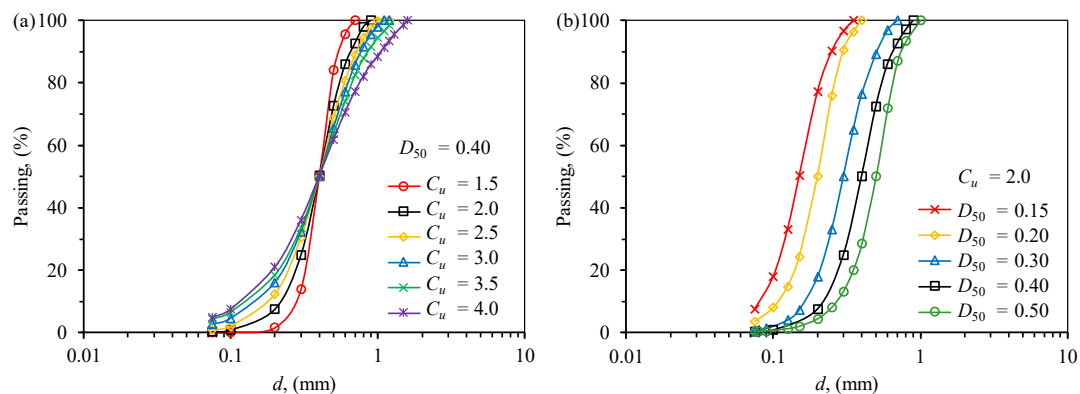


Figure 3. Grain size distributions of the spherical particles: (a) Group A; (b) Group B.

Table 1. Properties of the numerical samples.

Material Groups	C_u	D_{50} (mm)	φ
A	1.5, 2, 2.5, 3, 3.5, 4	0.4	0.36
B	2	0.15, 0.2, 0.3, 0.4, 0.5	0.36
C	2	0.4	0.36, 0.38, 0.4, 0.42

It is important to note two key aspects of the numerical setup. First, the DEM-generated particles are perfectly spherical, and thus the effects of particle angularity and surface roughness are not considered in this study. This simplification allows for a controlled investigation into the specific effects of grain size distribution, density, and contact angle. Second, while the Lvca-PMM framework is designed to incorporate locally variable contact angles [21], a uniform contact angle value is assigned to the solid phase for each simulation in this parametric study to clearly isolate its macroscopic effect.

3. Results and Discussion

3.1. Soil–Water Characteristic Curves

The simulated data and corresponding best-fit soil–water characteristic curves (SWCCs) for all investigated samples are presented in Figures 4 and 5, systematically illustrating the effects of variations in C_u , D_{50} , φ , and θ . As clearly demonstrated in the figures, the SWCCs exhibit a consistent leftward shift with decreasing C_u values and increasing D_{50} , φ , and θ . This trend aligns well with established experimental findings. For instance, the reduction in θ with increasing D_{50} and φ has been consistently reported in laboratory tests on sandy soils [13,35]. The observed influence of the contact angle is also in qualitative agreement with experimental studies that used liquids of different wettability [16,29].

A comparative analysis of the parameter influences reveals that D_{50} (Figure 4c,d) and θ (Figure 5) exert substantially more pronounced effects on the SWCC response compared with C_u (Figure 4a,b) and φ (Figure 4e,f). Particularly noteworthy is the nonlinear relationship observed between D_{50} variations and SWCC shifts. As evident in Figure 4c,d, while D_{50} increases by a constant increment of 0.1 mm, the resulting differences between adjacent SWCCs demonstrate significant nonlinear behavior. Specifically, the separation between curves for $D_{50} = 0.5$ mm and $D_{50} = 0.4$ mm is markedly smaller than that observed between $D_{50} = 0.4$ mm and $D_{50} = 0.3$ mm, which in turn is less pronounced than the distinction between $D_{50} = 0.3$ mm and $D_{50} = 0.2$ mm.

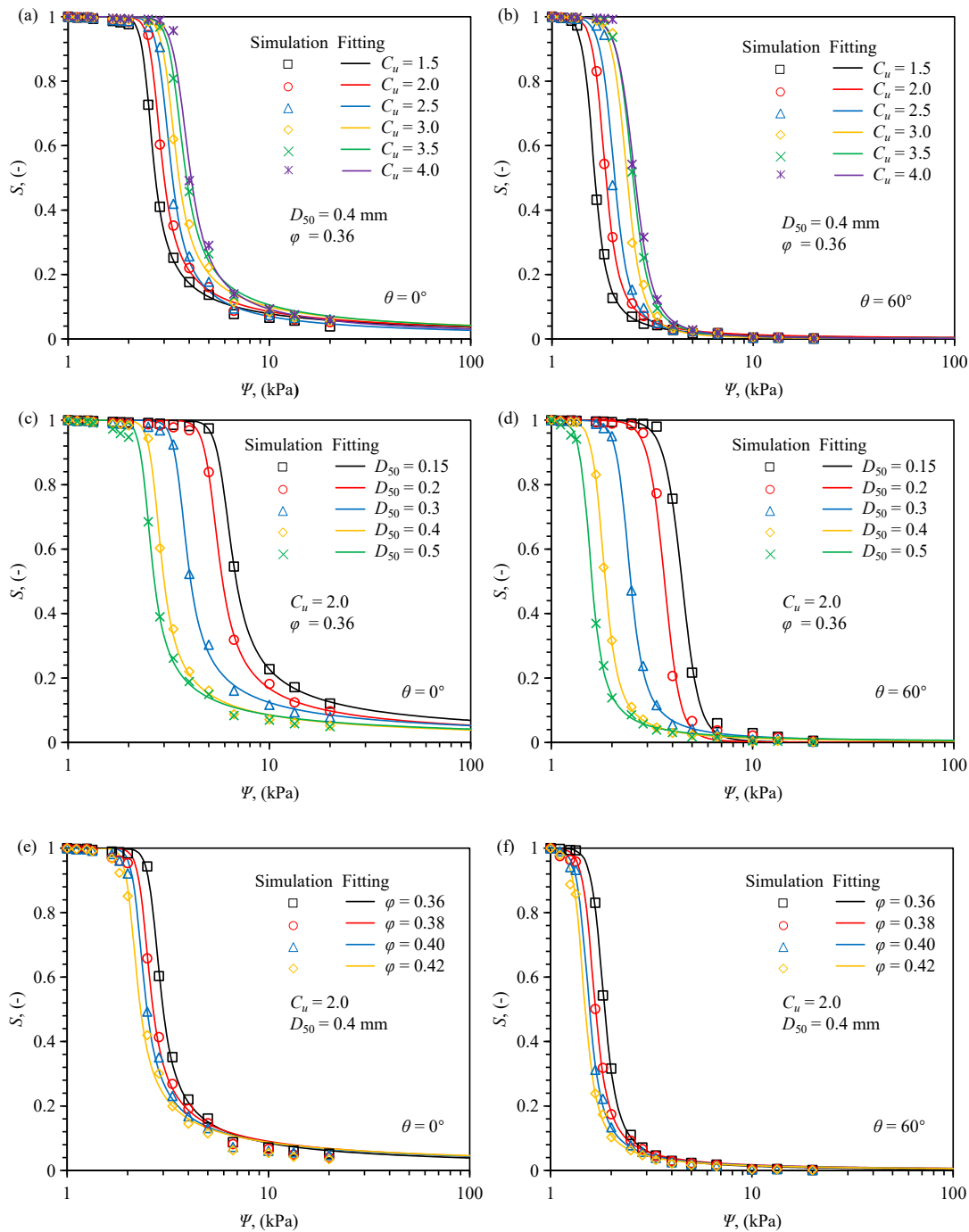


Figure 4. SWCCs of the samples for different C_u (a,b), D_{50} (c,d), ϕ (e,f) with $\theta = 0^\circ$ and 60° .

Regarding contact angle effects, the minimal distinction between SWCCs at $\theta = 0^\circ$ and $\theta = 20^\circ$ in Figure 5 can be attributed to the nearly identical radii of the digital spheres (r') calculated using Equation (2) for these two contact angle values, resulting in comparable solid phase dilation effects in the simulations. To provide more quantitative insights into these observed differences, subsequent sections will present detailed comparative analyses of key SWCC parameters, including Ψ_a and Ψ_r , offering numerical characterization of the parameter influences identified in this graphical analysis.

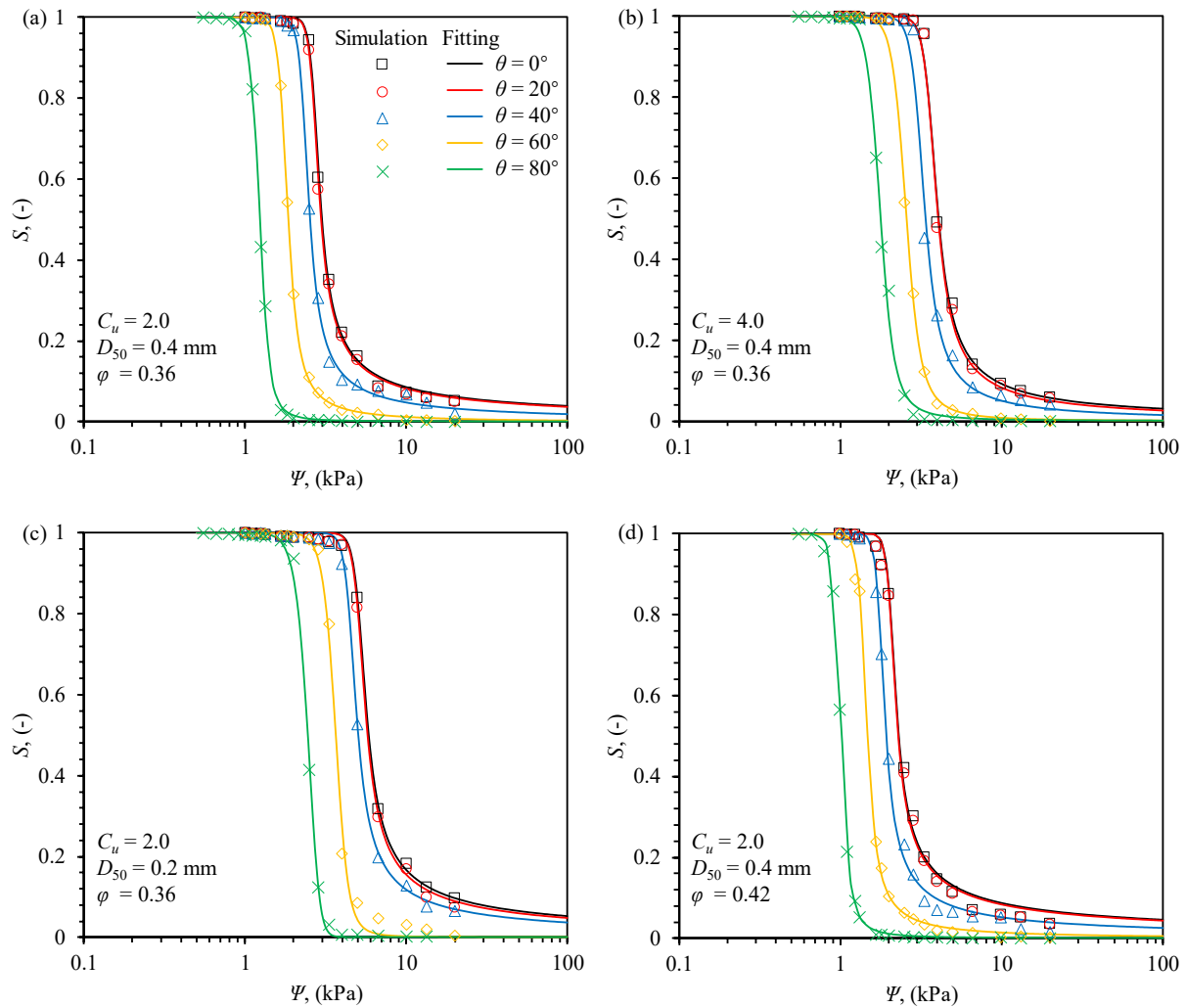


Figure 5. The effect of θ on the SWCCs of the sample with (a) $C_u = 2.0$, $D_{50} = 0.4$ mm, and $\phi = 0.36$; (b) $C_u = 4.0$, $D_{50} = 0.4$ mm, and $\phi = 0.36$; (c) $C_u = 2.0$, $D_{50} = 0.2$ mm, and $\phi = 0.36$; (d) $C_u = 2.0$, $D_{50} = 0.4$ mm, and $\phi = 0.42$.

3.2. The Effect of C_u on SWCC

Figure 6a and Figure 6b present the variations of Ψ_a and Ψ_r with respect to C_u , respectively. Both Ψ_a and Ψ_r increase with the increase in C_u , suggesting that the steeper the grain size distribution curve the stronger the water retention capacity (see Figure 4a,b). This occurs because fine particles in well-graded soils occupy the voids between larger particles, resulting in a reduction in overall pore size and an increase in pore size heterogeneity. The simulation results are consistent with experimental tests [13,38]. Both SWCC variables (Ψ_a and Ψ_r) show a linear relationship with C_u for any given θ . A linear equation of the form $y = aC_u + b$ is used to fit the SWCC variables with C_u , with the fitting parameters a and b , along with their respective R^2 values, are provided for each curve. Both the values of a and b in Figure 6b are larger than in Figure 6a, indicating Ψ_r is more sensitive than Ψ_a to changes in C_u . Generally, as θ increases, both the absolute values of a and b are decreased, as shown in Figure 6a,b. In other words, the steeper the slope of grain size distribution curve the less vulnerable the Ψ_a and Ψ_r on the contact angle.

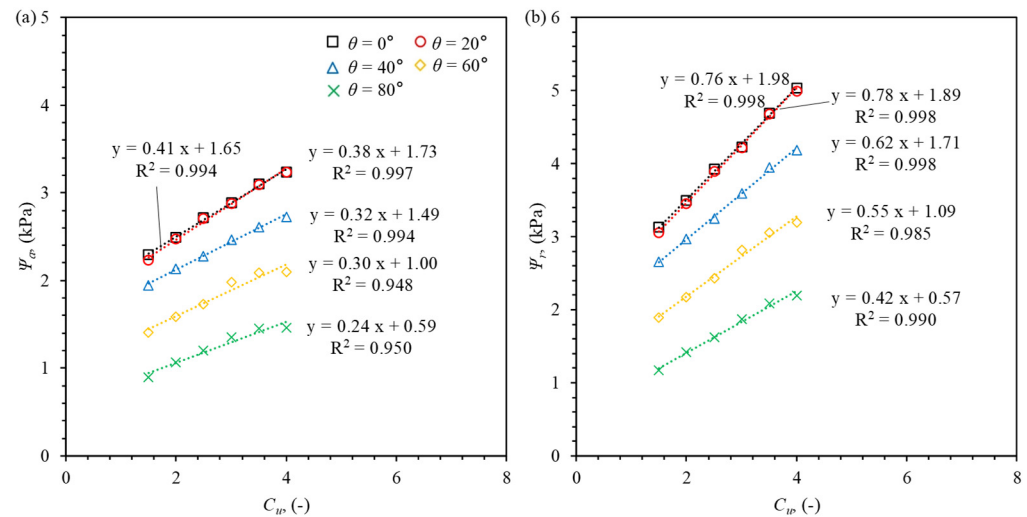


Figure 6. The effect of C_u on Ψ_a (a) and Ψ_r (b) of the SWCC for sample Group A.

3.3. The Effect of Grain Size on SWCC

Figures 7a and 7b show the relationships between Ψ_a and Ψ_r of the SWCCs for sample Group B, respectively. As D_{50} increases, both Ψ_a and Ψ_r decrease, indicating that, with the increase in grain size, pore sizes become larger, leading to the lower water retention capacity. This tendency that Ψ_a and Ψ_r decrease with increasing D_{50} is in consistent with experimental results [13,14,38]. A clear linear relationship between SWCC variables (Ψ_a and Ψ_r) and D_{50} in the log–log space can be observed in Figure 7, indicating that the variables (Ψ_a and Ψ_r) follow a power-law trend. The power-law relationship between Ψ_a and D_{50} was also reported in experimental observations [14]. Hence, the data are fitted with power-law equations in the form $y = aD_{50}^b$. Where parameter a represents the intercept in the log–log space, which corresponds to the value of y (i.e., Ψ_a and Ψ_r) when $D_{50} = 1$ mm, b represents the slope of the curve in the log–log space. The fitting parameters a and b , along with their respective R^2 values, are provided for each curve, demonstrating an excellent fit across all conditions ($R^2 > 0.99$).

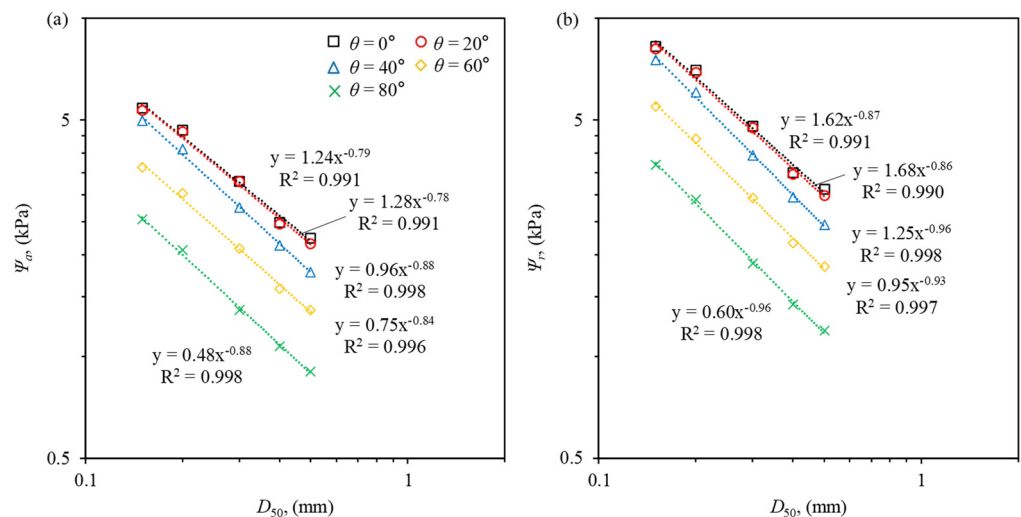


Figure 7. The effect of D_{50} on Ψ_a (a) and Ψ_r (b) of the SWCC for sample Group B.

With the increase in θ , both Ψ_a and Ψ_r increase, which means that SWCC shift leftwards in higher contact angle scenarios. In Figure 7a,b, the parameter a decreases as θ increases, indicating that the magnitudes of Ψ_a and Ψ_r become smaller at higher contact angles. Slope b becomes more negative with increasing θ , showing that the rate of decrease in Ψ_a and Ψ_r

with D_{50} is more pronounced at larger θ . The separation between the curves in Figure 7a,b becomes more significant at smaller D_{50} , highlighting a stronger influence of θ at finer particle sizes. For the same contact angle, however, parameter a in Figure 7b is larger than Figure 7a as expected, as the residual suction is larger than the air entry value. Slope b in Figure 7a is larger than Figure 7b, indicating that the impact of D_{50} on Ψ_a is less significant than on Ψ_r .

Figure 8 presents the effect of D_{10} on the Ψ_a and Ψ_r of the SWCC of the sample Groups A and B. The change in SWCC variables (Ψ_a and Ψ_r) with respect to D_{10} also exhibit a power-law trend, similar to that observed for D_{50} in Figure 7. For the same sample Group B, as the range of D_{10} (0.08 mm to 0.271 mm) is narrower than the range of D_{50} (0.15 mm to 0.5 mm), the values of intercept a in Figure 7a,b are larger than Figure 8c,d, as expected. However, it is interesting to note that the values of slope b almost remain constant in Figures 7a,b and 8c,d. The parameters a and b for Group A in Figure 8a,b exhibit a similar trend with respect to θ as for Group B in Figure 8c,d. With the increase in θ , both a and b decrease for Ψ_a and Ψ_r . However, the values of a and b are quite different for Groups A and B, as the values of C_u are different. For example, a and b for Ψ_a in Figure 8a range from 1.44 to 0.47 and from -0.37 to -0.53 , respectively, while in Figure 8d, a and b vary between 0.81 to 0.29 and between -0.76 to -0.87 , respectively. This observation suggests that D_{10} alone cannot explain the variation of SWCC, and the conjoint effect of C_u cannot be overlooked.

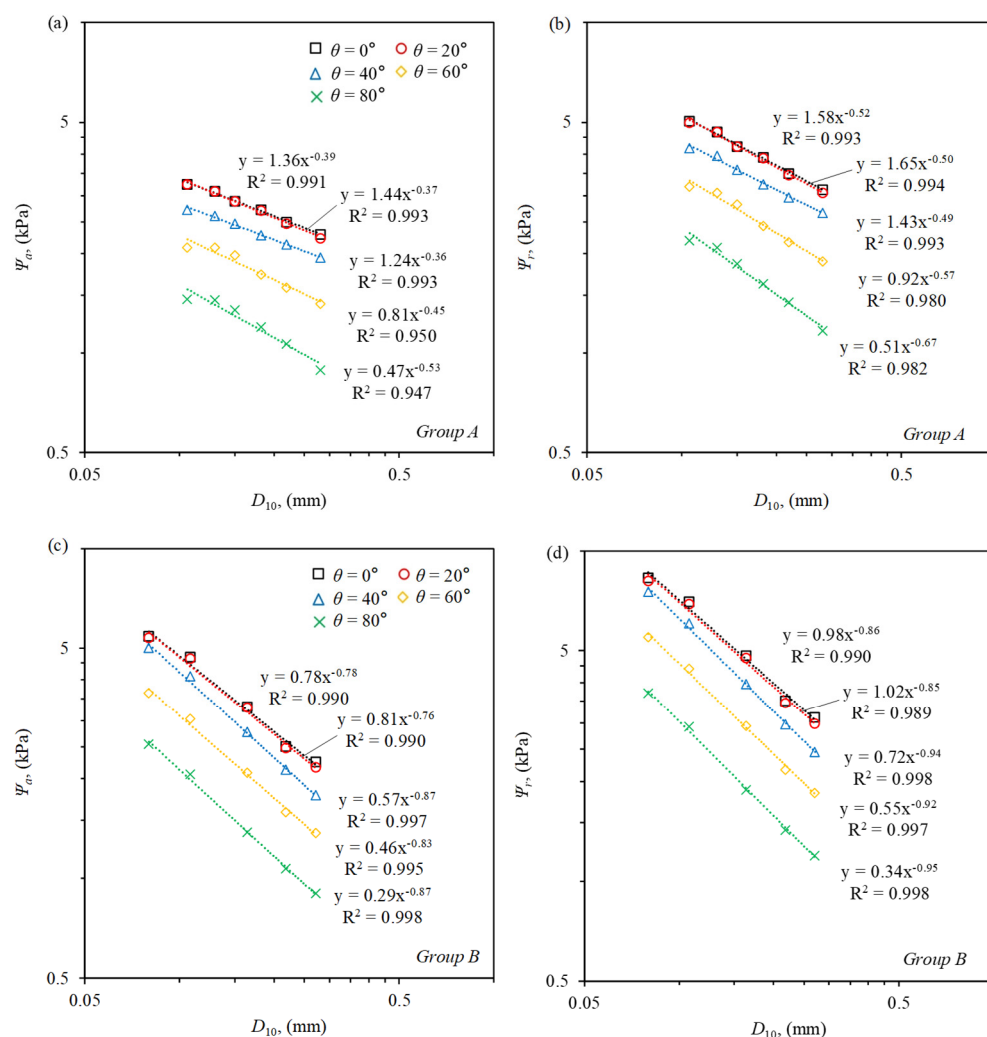


Figure 8. The effect of D_{10} on Ψ_a and Ψ_r of the SWCC for samples: (a,b) Group A; (c,d) Group B.

3.4. The Effect of ϕ on SWCC

Figures 9a and 9b show the variations of Ψ_a and Ψ_r as a function of ϕ , respectively. With the increase in ϕ , both Ψ_a and Ψ_r decrease, which is in agreement with the experimental findings [13]. Both Ψ_a and Ψ_r show a linear relationship with ϕ for any given θ . The data are fitted with a linear equation of the form $y = aC_u + b$. The fitting parameters a and b , along with their respective R^2 values, are provided for each curve. Both the values of a and b in Figure 9b are larger than in Figure 9a, indicating that the sensitivity of Ψ_r to ϕ is greater than that of Ψ_a . Generally, as θ increases, both the absolute values of a and b are decreased, as shown in Figure 9a,b.

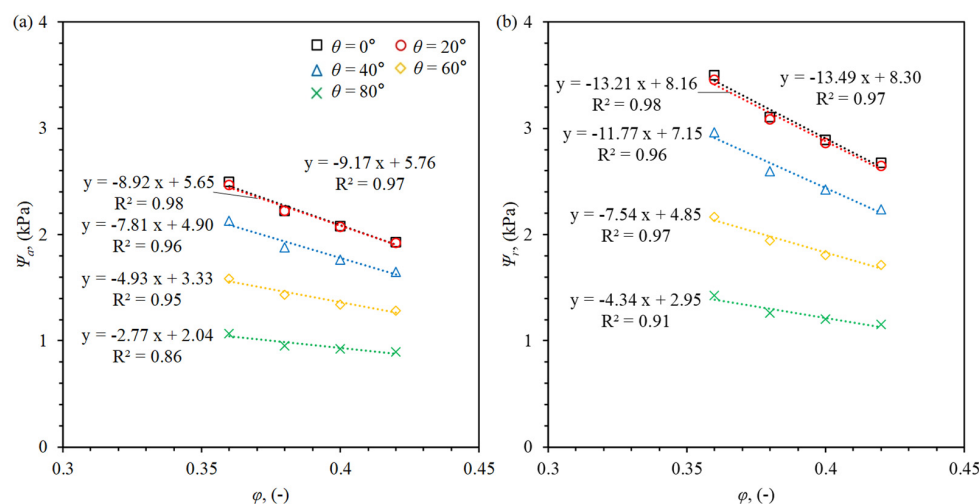


Figure 9. The effect of ϕ on Ψ_a (a) and Ψ_r (b) of the SWCC for sample Group C.

3.5. The Effect of θ on SWCC

The effects of θ on Ψ_a and Ψ_r for different samples are shown in Figure 10. Across all three groups of samples, the relationships between these SWCC variables and $\cos(\theta)$ are consistently linear. Both Ψ_a and Ψ_r exhibit positive correlations with $\cos(\theta)$ in all groups, suggesting that a smaller contact angle (higher $\cos(\theta)$) enhances the soil's ability to retain water. With the increase in C_u and the decrease in D_{50} and ϕ , Ψ_a and Ψ_r show stronger increases with $\cos(\theta)$. D_{50} has the strongest influences on the relationship between SWCC variables (Ψ_a and Ψ_r) and $\cos(\theta)$ compared with C_u and ϕ . In summary, while the general linear trends between SWCC parameters and $\cos(\theta)$ are consistent across Groups A, B, and C, the magnitude of the responses depend on the specific soil structural properties being varied. These findings highlight the interplay between contact angle and soil characteristics in determining the SWCC behavior.

3.6. Curve Fitting

Both the SWCC variables (Ψ_a and Ψ_r) exhibit a linear relation with respect to C_u , ϕ , and $\cos(\theta)$, as shown in Figure 6, Figure 9, and Figure 10, respectively. While a power function in the form of $y = aD_{50}^b$ can be used to fit the three variables with respect to D_{50} , as shown in Figure 7, parameter b changes slightly with the variation of θ . By acknowledging these relationships between SWCC variables and the soil characteristics, a power-like function is used to fit each of the datasets. The resulting functions are presented in Equations (6) and (7), with the signs of the coefficients reflecting the positive and negative impact of the respective variables (C_u , ϕ , D_{50} , and $\cos(\theta)$). The comparison between the predicted SWCC variables (Ψ_a^{pred} and Ψ_r^{pred}) by Equations (6) and (7) and the respective simulated data, along with their respective R^2 values, is shown in Figure 11. The predicted SWCC variables match very well with the simulated data (see the values of R^2). As shown in

Figure 11a,b, the expands of Ψ_a and Ψ_r for Group B are the widest, indicating that D_{50} has a larger influence on Ψ_a and Ψ_r , while the expands of Ψ_a and Ψ_r for Group C are the narrowest, reflecting that the impact of φ on SWCC is smaller than C_u and D_{50} . Although φ has the biggest coefficient in Equations (6) and (7), the variation range of φ for sand is very narrow, generally between 0.2 and 0.5.

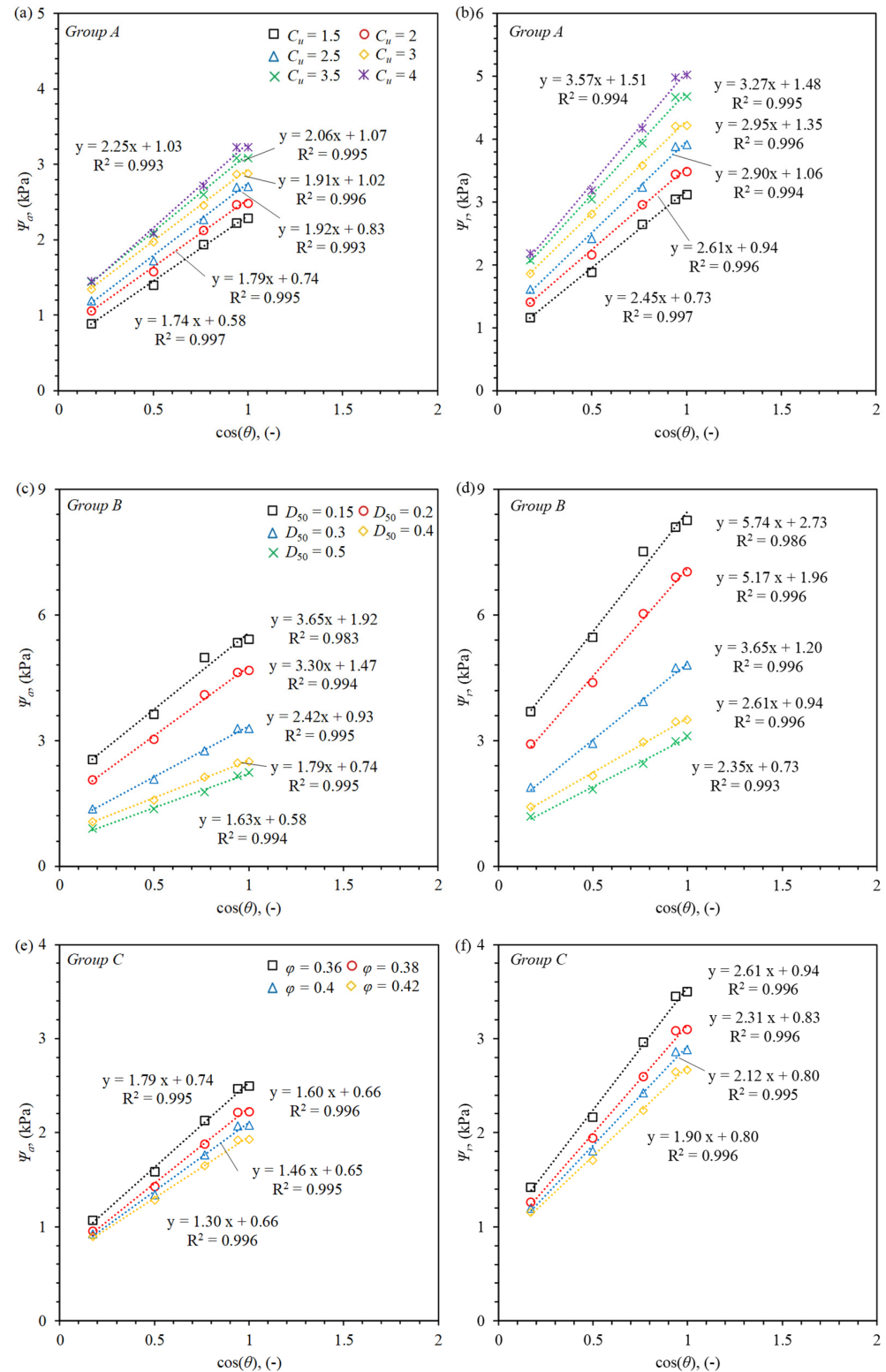


Figure 10. The effect of θ on Ψ_a and Ψ_r of the SWCC for samples: (a,b) Group A; (c,d) Group B; (e,f) Group C.

$$\Psi_a = [0.142C_u - 3.877\phi + 0.831\cos(\theta) + 1.483]D_{50}^{-0.825} \quad (6)$$

$$\Psi_r = [0.257C_u - 5.544\phi + 1.148\cos(\theta) + 1.923]D_{50}^{-0.901} \quad (7)$$

Figure 12a and Figure 12b show the results of applying Equation (6) and Equation (7) to predict the values of Ψ_a and Ψ_r , respectively, for a collection of experimental data by Sakaki et al. [14] and Alves et al. [27]. Ψ_a for a wide range of silica sand was measured in Sakaki et al. [14]. For the tested sand materials, $D_{50} = 0.1 \sim 1.5$ mm, $C_u = 1.1 \sim 5.6$, and $\phi = 0.24 \sim 0.44$, the contact angle θ is assumed to be zero [14]. The drying SWCC data for the glass beads were reported in Alves et al. [27]. The Fredlund and Xing equation (Equation (5)) was used in this study to fit the measured data in Alves et al. [27], and Ψ_a and Ψ_r were determined using the method shown in Figure 5. For the EU-165 tested with Triton X-100 (EU-165 X-100, $\gamma = 3.28 \times 10^{-2}$ N/m) and sodium chloride (EU-165 NaCl, $\gamma = 7.97 \times 10^{-2}$ N/m) aqueous solutions, Ψ_a and Ψ_r are modified by a scale factor γ_0/γ_1 , where γ_0 and γ_1 are the respective surface tension values of the reference solution (e.g., water) and the solution of interest [39]. Properties of the materials and the predicted Ψ_a and Ψ_r are summarized in Table 2. As shown in Figure 12, the proposed empirical functions perform reasonably well when predicting Ψ_a and Ψ_r for coarse granular materials.

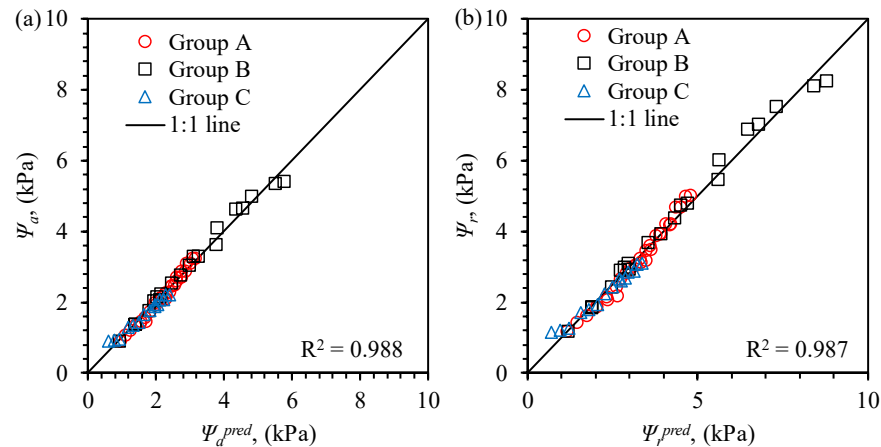


Figure 11. Comparison between the function predicted and simulated: (a) Ψ_a ; (b) Ψ_r .

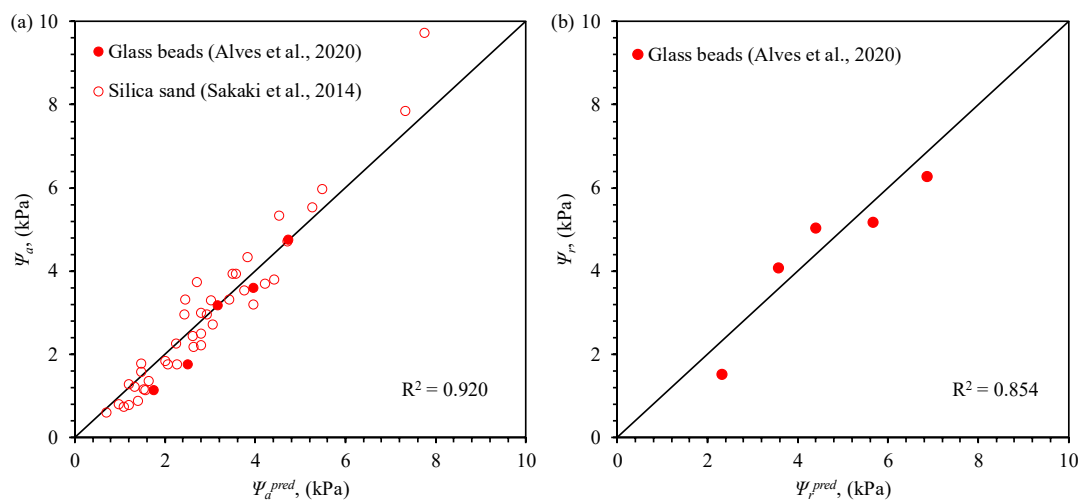


Figure 12. Comparison between the estimated and measured (a) Ψ_a and (b) Ψ_r . Experimental data for the glass beads and silica sand were obtained from Alves et al. [27] and Sakaki et al. [14], respectively.

Table 2. Air entry values and residual suctions.

Material Type		$D_{50}(\text{mm})$	C_u	φ	θ ($^{\circ}$)	$\Psi_a(\text{kPa})$	$\Psi_a^{pred}(\text{kPa})$	$\Psi_r(\text{kPa})$	$\Psi_r^{pred}(\text{kPa})$
Glass beads †	EU-165 Nacl	0.165	1.06	0.354	56.5	3.172	3.178	5.032	4.395
	EU-165 X-100	0.165	1.06	0.354	12.6	4.743	4.736	6.263	6.865
	EU-165	0.165	1.06	0.354	39.8	3.592	3.973	5.182	5.655
	WG	0.368	1.92	0.334	39.8	1.755	2.505	4.080	3.561
	EU-412	0.412	1.06	0.368	39.8	1.127	1.755	1.519	2.306
Group A ‡ uniform crushed silica	A1	1.51	1.7	0.4	0	0.589	0.716	-	-
	A2	0.95	1.6	0.41	0	0.785	0.994	-	-
	A3	0.72	1.4	0.41	0	1.275	1.212	-	-
	A4	0.56	1.4	0.41	0	1.570	1.491	-	-
	A5	0.5	1.3	0.43	0	1.766	1.474	-	-
	A6	0.31	2	0.43	0	2.943	2.449	-	-
	A7	0.2	1.7	0.42	0	3.924	3.502	-	-
Group B ‡ uniform round silica	B1	1.04	1.2	0.32	0	0.765	1.205	-	-
	B2	0.75	1.2	0.32	0	1.128	1.578	-	-
	B3	0.52	1.2	0.33	0	1.746	2.068	-	-
	B4	0.36	1.2	0.33	0	2.207	2.801	-	-
	B5	0.27	1.2	0.34	0	3.306	3.437	-	-
	B1'	1.08	1.2	0.34	0	0.726	1.095	-	-
	B2'	0.75	1.2	0.33	0	1.148	1.529	-	-
	B3'	0.53	1.1	0.33	0	1.825	2.012	-	-
Group C ‡ uniform med-fine silica	B4'	0.36	1.2	0.33	0	2.482	2.801	-	-
	C1	0.28	1.7	0.32	0	3.532	3.761	-	-
	C2	0.12	1.7	0.33	0	7.848	7.344	-	-
Group D ‡ less-uniform crushed silica	C3	0.1	1.7	0.36	0	9.722	7.759	-	-
	D1	0.45	2	0.37	0	2.256	2.251	-	-
	D2	0.41	2.9	0.38	0	2.433	2.617	-	-
	D3	0.15	1.9	0.37	0	5.964	5.504	-	-
	D4	0.19	2.2	0.38	0	5.317	4.544	-	-
	D5	0.42	5.4	0.31	0	4.326	3.849	-	-
	D6	0.3	2.5	0.4	0	3.296	3.023	-	-
Group E ‡ less-uniform round silica	D7	0.68	1.7	0.41	0	1.207	1.329	-	-
	E1	0.85	1.4	0.33	0	0.863	1.411	-	-
	E2	0.75	1.6	0.32	0	1.354	1.650	-	-
	E3	0.6	2.1	0.29	0	1.756	2.269	-	-
	E4	0.52	2.2	0.28	0	2.178	2.645	-	-
	E5	0.43	4.2	0.24	0	3.188	3.977	-	-
	E6	0.36	3.6	0.26	0	3.679	4.226	-	-
	E7	0.31	3.2	0.28	0	3.796	4.427	-	-
	E8	0.27	2.9	0.29	0	4.709	4.722	-	-
Group F ‡ field sands	E9	0.22	2.8	0.31	0	5.523	5.271	-	-
	F1	0.3	2.8	0.44	0	3.728	2.720	-	-
	F2	0.2	1.3	0.4	0	3.934	3.579	-	-
	F3	0.34	2.1	0.35	0	2.717	3.060	-	-
	F4	0.32	1.8	0.38	0	2.982	2.810	-	-

† Data for glass beads are extracted from Alves et al. [27]. ‡ Data for silica and field sands are obtained from Sakaki et al. [14].

4. Conclusions and Limitations

This study provides a comprehensive investigation into the effects of grain size distribution, density, and contact angle on the soil–water characteristic curve (SWCC) of coarse granular materials using the Lvca-PMM model. By integrating the DEM to generate granular material samples and applying the Lvca-PMM approach, this research provides a detailed understanding of how C_u , D_{50} , φ , and θ influence SWCC behavior and key variables such as Ψ_a and Ψ_r . Some main conclusions can be summarized as follows:

1. The results demonstrate that smaller C_u , larger D_{50} , higher φ , and increased θ result in a leftward shift of the SWCC curve, leading to lower Ψ_a and Ψ_r . These results align closely with experimental observations, which validate the predictive capability of the Lvca-PMM model.
2. Linear relationships were identified between SWCC variables (Ψ_a and Ψ_r) and factors such as C_u , φ , and $\cos(\theta)$. In contrast, a power-law relationship was observed between SWCC variables and D_{50} , demonstrating the nonlinear effects of grain size distribution on water retention behavior, particularly for finer particle sizes.
3. Empirical equations developed in this study provide practical tools for estimating Ψ_a and Ψ_r based on soil properties. These equations demonstrate that the combined effects of grain size distribution, density, and contact angle must be considered to accurately predict SWCC behavior.

The findings and empirical models presented in this work offer significant practical value for researchers and engineers working in unsaturated soil mechanics, geotechnical design, and hydrological modeling. The proposed equations (Equations (6) and (7)) enable efficient estimation of key SWCC parameters (Ψ_a and Ψ_r) without the need for time-consuming laboratory tests, especially for coarse-grained soils. This is particularly useful in the preliminary design stages of granular fills, drainage systems, and soil stabilization projects. Moreover, the explicit incorporation of the contact angle effect provides a more realistic representation of field conditions where soil wettability may vary due to environmental factors or contamination. The Lvca-PMM framework also serves as a reliable numerical tool for simulating multiphase flow in porous media, supporting further research into fluid transport mechanisms in variably saturated soils.

While this study provides valuable insights into the SWCC of coarse-grained materials, several limitations warrant discussion. The use of spherical particles precludes replication of the enhanced water retention capacity characteristic of angular soils, where finer pores associated with particle asperities and more complex pore throats lead to higher air entry values and residual suctions [40], making the proposed empirical models (Equations (6) and (7)) most applicable to coarse-grained materials with rounded particles. Furthermore, it is important to note that natural soils exhibit inherent fabric anisotropy arising from their deposition history, stress path, and heterogeneous particle shapes [41–43], all of which critically govern their hydraulic and mechanical response. Hence, our model's assumption of statistically isotropic fabric provides only a baseline understanding for isotropic packings. Additionally, the current implementation of the Lvca-PMM framework is developed and validated specifically for simulating the primary drainage process. It does not capture the wetting process or the associated hydraulic hysteresis observed in real soils under cyclic drying and wetting. Extending the Lvca-PMM to simulate wetting scans is a recognized challenge that involves incorporating additional physics, such as criteria for pore filling during imbibition (e.g., snap-off) and spatially variable receding/advancing contact angles. Future research should therefore focus on incorporating realistic particle shapes, exploring anisotropic fabric effects guided by X-ray tomography studies [41–43], and extending the Lvca-PMM framework to simulate wetting scans and hysteresis.

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