Abstract: Controlled delivery of water to plant root zone remains a challenge in the exploration of plant growth under zero gravity, in which soil water retention characteristics are difficult to predict due to possible soil particle rearrangement and pore restructuring. This paper aims to provide an understanding of the effect of soil particle rearrangement on the water retention characteristics in zero gravity. A three-dimensional pore network model is developed to predict water retention characteristics under two forms of particle packing—cubic packing (most porous) and rhombohedral packing (most compact). The pore-throat distributions, as input parameters to the network model, are derived from particle size distribution under the two forms of particle arrangement. The model simulations reveal the quantitative variation of water retention characteristics due to particle rearrangement. Soil particle rearrangement that occurs during the drying process is shown to significantly change the water retention curve when a soil is near saturation. When the soil is near residual water content, the particle rearrangement has little effect on the water retention curve. The model results indicated that an increase in packing density results in decreased water content at saturation, increased bubbling pressure, and accentuated water retention hysteresis. The model also reveals nonuniform spatial distribution of pore fluid in porous medium in zero gravity. Although this paper studied the soil-water characteristics from the microgravity perspective, its results also contribute to the understanding of the soil-water characteristics due to soil compaction on Earth.

DOI: 10.1061/(ASCE)1532-3641(2009)9:4(179)

CE Database subject headings: Vegetation; Soil water; Soil compaction; Particles.

Introduction

One of the challenges facing plant growth under zero or reduced gravity is the controlled delivery of water to the plant root zone. In a microgravity environment, the location or distribution of water in soils is less predictable and can easily lead to localized overmoistening (Hoehn et al. 2000). Analyses of the experimental results on the spaceflights ASC-1 and Greenhouse-2 suggest that density, pore-size distribution, and water transport properties change in microgravity (Jones and Or 1999). The recent experiments conducted aboard KC-135 microgravity flight (Reddi et al. 2005) also revealed particle separation and rearrangement. The pore-size variability and pore restructuring lead to water retention variation and make the precise control of water content difficult (Steinberg et al. 2005a). How the water retention and distribution change from 1g to 0g, as a result of rearrangement of soil particles and pore structure in 0g, is the primary focus of this paper.

Soil water retention characteristic is a basic soil-water relation-
tion (Lowry and Miller 1995; Reeves and Celia 1996; Peat et al. 2000; Ahmadi et al. 2001). With the same particle size distribution, the pore-size distribution can vary due to compaction, vibration, and particle rearrangement that the soil experiences during and after a shuttle launch. A single specified probability function might not account for the pore-size distribution variation. Arya and Paris (1981) proposed a model to predict the moisture characteristic of a soil from its particle size distribution, bulk density, and particle density. In their model, pores were idealized as cylindrical capillary tubes, and pore sizes were derived from particle sizes. In the derivation of pore sizes, an empirical constant ($\alpha$) was used based on experimental WRC and it fell in a narrow range (1.35–1.40) for a loam and silty clay soils. Although the approach by Arya and Paris (1981) related the pore-size distribution with particle size distribution and soil compaction, the extension of the empirical constant ($\alpha$) to granular soils that were often used as plant growth media in space needs further verification.

In order to provide an understanding of the effect of particle rearrangement on water retention characteristics under microgravity, a three-dimensional pore network model is developed in this study. The pore-size distributions are represented using the pore-throat distributions, which are derived from particle size distribution based on two extreme particle arrangements (the most compact and the most porous spherical packing). The model is then used to reveal the variation of water retention characteristics and the spatial distribution of pore fluid due to particle rearrangements. The soil water characteristic curve (SWCC) is also the key unsaturated soil property when solving problems using unsaturated soil mechanics, such as seepage, air, and heat flow in soils, shear strength, and stress-deformation relationship (Fredlund 2006). The 3D pore network model presented in this paper studies the effect of particle packing on SWCC in terms of matric suction versus water content. Under microgravity, matric suction is applied externally when controlling the water in a plant growth module; while in the terrestrial condition, matric suction in soil is usually realized by gravity. Although this paper studied the SWCC from the microgravity perspective, its results also contribute to the understanding of the soil-water characteristics due to soil compaction on Earth.

**Model Development**

**Model Formulation**

A three-dimensional pore network model is developed based on a two-dimensional network model proposed by Payatakes et al. (1973), Ng et al. (1978), and Payatakes et al. (1980). In a porous medium, an irregular pore can be idealized as a pore body with pore throats. In this model, a pore is represented using a unit cell shown in Fig. 1(a). The wall profile of a unit cell is assumed to follow sinusoidal function. The pore body diameter ($a$), the pore length ($h$), and the volume of the unit cell ($V_{UC}$) can be calculated using the pore throat diameter ($d$). The formulae were presented by Payatakes et al. (1980).

The pore network is made of three-dimensional elemental pores, namely, *conceptual elemental void space* (CEVS) as shown in Fig. 1(b). Each CEVS consists of six half unit cells in the three dimensions. The six half unit cells in a CEVS can have different sizes, and together they make up one 3D conceptual pore. A CEVS is the smallest unit in the network and the CEVSs are interconnected with each other via pore throats. Two neighboring CEVSs share the same pore throat. Fig. 2 shows a 3D pore network model with dimension of $2 \times 2 \times 2$ CEVSs. Given the particle size distribution, pore-throat distribution, porosity, and the particle density of a porous medium, the pore network uniquely represents the pore structure of the porous medium. It is worth mentioning that the CEVS is a different concept from the representative elemental volume (REV) used by Nitao and Bear (1996) and Reddi et al. (2000). REV is the smallest entity that possesses the representative physical properties of an entire porous medium, while CEVS in this study is an idealized three-dimensional pore. One REV could comprise more than one CEVS.

**Pore-Size Distribution in Network Model**

The dimension of pores, including pore body and pore throat, depends on particle sizes and arrangement (or packing). Packing of spheres has two extreme cases: cubic packing [Fig. 3(a)] and rhombohedral packing [Fig. 4(a)]. Cubic packing is the most porous packing of uniform spheres with porosity of 0.47; rhombohedral packing is the most compact packing of uniform spheres with porosity of 0.26. Fig. 3(b) shows the pore throat formed by

![Fig. 1. 3D pore network model configuration: (a) unit cell simulating pore; (b) 3D conceptual elemental void space (CEVS)](image)

![Fig. 2. 3D pore network model of dimension of $2 \times 2 \times 2$ CEVS (conceptual elemental void space)](image)
uniform spheres of diameter $D$ in cubic packing. The pore throat diameter ($d$), represented by segment $EF$, can be calculated from the particle diameter

$$d = 0.4142D$$  \hspace{1cm} (1)$$

Fig. 4(b) shows the pore throat formed by uniform spheres with diameter $D$ in rhombohedral packing. The pore throat radius is represented by segment $OP$, because $OP$ is the smallest restriction in the void formed by the three spheres. The pore throat diameter ($d$) can be calculated using (Villaume 1985)

$$d = 0.1547D$$  \hspace{1cm} (2)$$

Using Eq. (1) or (2), the pore throats can be calculated from particle size distribution. This study uses Ottawa sand, whose particle size distribution is shown in Fig. 5. The size range of the Ottawa sand is similar to that of a baked ceramic aggregate material (0.25–1.0 mm) (also shown in Fig. 5), which was previously used as a plant growth medium in spaceflight (Steinberg et al. 2005b). Ottawa sand typically consists of 99.8% SiO$_2$ (quartz) and trace amounts of metal oxides, is spheroidal, and has rough surface. To calculate the volumetric percentage of pores, the particle size distribution is first converted into a differential distribution. The accumulative volume ($V^p_d$) of all the pores with pore throats of diameter $d$ is calculated using

$$V^p_d = \frac{M_D e}{\rho}$$  \hspace{1cm} (3)$$

where $M_D$=mass of particles of diameter $D$ that form the pore throats of diameter $d$; $\rho$=particle density (2.65 g/cm$^3$ for Ottawa sand); and $e$=void ratio, which can be calculated using porosity. It is assumed that the void ratio for each group of particles of size $D$ has the same value as the void ratio of the entire sand sample. The calculation of pore throat is an approximation because pore throats are naturally formed by particles of various sizes. Since this paper focuses on the variation range of WRC due to particle rearrangement, this method gives the smallest and largest possible pore throat distributions. Fig. 6 shows the derived pore-throat distributions of cubic and rhombohedral packing of Ottawa sand, in terms of pore throat diameter versus volumetric percentage ($V^p_d$) of pores with pore throat diameter $d$. Since the pore-throat distributions are derived from the discrete particle size distribution, the pore throat diameters have discrete values, as shown in Fig. 6. The actual pore throat diameter may be continuous and the pore-throat distributions used in this model are only approximation. The pore network is initialized using the pore-throat distribution. In a network with given array dimensions (in terms of number of CEVS), the total number of pore throats is known. The volumetric percentage ($V^p_d$) in a pore-throat distribution is first converted to numeric percentage ($N^p_d$) of pore throats
2. Rewetting process:

where

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lows:

fore, the capillarity in the pore body throughout

fluid reaches residual saturation. If suction is then reduced, the
growth to the plant roots—“Haines jump” (Haines 1930), and the fluid in the entire pore is assumed to instantly vacate the pore, a phenomenon often referred to as “piston drainage.” As the suction pressure increases, it gradually overcomes higher capillary pressures corresponding to smaller pore throats, and pore fluid continues to drain from smaller pores until the pore fluid reaches residual saturation. If suction is then reduced, the rewetting process starts. Water first enters the smaller pores where capillary pressure is higher and can overcome the external suction. In order for water to enter a pore, the capillary pressure throughout the pore has to overcome the external suction. Therefore, the capillarity in the pore body (the smaller capillary pressure) dictates the rewetting process.

The drying and rewetting processes are summarized as follows:

1. Drying process:

\[
\Delta p > p_c = \frac{4 \gamma \cos \theta_s}{d} \Rightarrow \text{water drains from the pore} 
\]  

The displacement of wetting fluid by nonwetting fluid (air in this case) is governed by pore throat of size \(d\); and

2. Rewetting process:

\[
\Delta p < p_r = \frac{4 \gamma \cos \theta_r}{d} \Rightarrow \text{water enters the pore} 
\]  

The displacement of nonwetting fluid (air in this case) by wetting fluid is governed by pore body of size \(d\). In the above formulae, \(\Delta p\) = external suction; \(\theta_r\) = receding contact angle; and \(\theta_a\) = advancing contact angle. Sklodowska et al. (1999) measured the contact angle of water on quartz, the value was \(32.79 \pm 1.12^\circ\). In this simulation, it is assumed that \(\theta_r = 33^\circ\) for Ottawa sand. Usually advancing contact angle is larger than receding contact angle. The ratios of the advancing contact angle to the receding contact angle of water on various materials are from 1.02 to 1.40 (Somundaran 2006). So a ratio of 1.2 is chosen, and the advancing contact angle of 40° is used in this study.

Hysteresis, which is the irreversible water retention phenomenon dependent on drying and rewetting processes, is modeled. Levine et al. (1977) generalized two types of hysteresis: contact angle hysteresis due to the different values of receding contact angle (in drying process) and advancing contact angle (in rewetting process), and capillary hysteresis due to the nonuniform cross section of pores. In this model, capillary hysteresis is simulated using Eqs. (7) and (8), and contact angle hysteresis is simulated by choosing different values of receding and advancing contact angles.

The sensitivity of modeling results to the network size is first studied. The simulation reveals that the modeling outputs converge when the network size is larger than \(10 \times 10 \times 4\), i.e., ten CEVs in both \(x\) and \(y\) directions and four CEVs in the \(z\) direction. The network size is then chosen to be \(30 \times 30 \times 5\) in the following simulations. Initially, all the pores are filled with water, then suction is applied downward at the bottom of the network. The top and side walls of the pore network are assumed to be impermeable, and water only drains or enters at the bottom. Water entrapment is considered during the drying process: if a water-filled pore is entirely surrounded by air-filled pores, it becomes hydraulically disconnected from the water sink, and the water in this pore cannot drain. The pore water is then entrapped and contributes to residual water content. Suction is increased at a 20 mm increment. At each suction, each CEV that is filled with water and is not completely isolated from the water sink is checked against drying process criterion, [Eq. (7)]. If the capillary pressure at any of the six pore throats that connect to a water-filled CEV satisfies Eq. (7), pore water in this CEV drains out. The process is repeated at each suction until the pore fluid in the entire network can no longer drain upon further increase in suction. Then the rewetting process starts by reducing the suction by a 20 mm decrement. At each suction, each CEV that is empty and has at least one neighboring CEV that is filled with water is checked against rewetting process criterion, [Eq. (8)]. The process is repeated at each suction until the pore network is saturated. Air entrapment is not considered in the rewetting process. The pressure of the air phase is assumed to always be atmospheric. In the simulations, gravity is ignored; only capillary force and external suction pressure are considered. In this model, it is assumed that matric potential is constant in the 3D pore network at certain suction, so that vertical water content distribution is constant. Under zero gravity, this assumption may be valid. Under 1g, this assumption introduces systematic error and yields smoothed water retention characteristic (Peters and Durner 2006).

The 3D network model also provides a useful tool in investigating the spatial distribution of pore fluid in porous media under zero gravity. Among the primary design requirements for water replenishment of plants in micro or zero gravity are the even distribution of water to plants and prevention of flooding to allow oxygen exchange to the plant roots (Scovazzo et al. 2001). In the 3D pore network, the locations of CEVs occupied by water can be determined, so the spatial distribution of pore fluid in the porous media can be visually presented during the drying and rewetting processes. In addition to the changes in gravitational force, plant growth modules are influenced by vibrations during the orbital movement of a spaceflight. Vibrations may cause soil
particles to shift from loose condition to compact condition or vice versa at the same suction, causing the spatial distribution of pore fluid to change accordingly. Also, root penetration in soil pores results in the compaction of soil and reduces pore space adjacent to root channels (Barley 1954). In this paper, the effect of particle rearrangement during the drying process on the water retention characteristics and pore fluid spatial distribution is explored.

It is noted that the network model does not consider adsorption (water accumulation on particle surface) and absorption (water diffusion into particles). The lack of consideration of adsorptive forces and liquid films was identified as a deficiency in current theories of transport and flow in porous media (Celia et al. 1995; Nitao and Bear 1996). The water held to solid due to sorption (including adsorption and absorption) contributes to the residual water content, which is insignificant in sandy soils (θ = 0.02 in the Ottawa sand, Fig. 7). In clays, sorption may result in a significant amount of water held to solids due to the diffuse double layer and the clay mineral structure.

Results and Discussion

**Experimental Water Retention Characteristics**

Water retention of Ottawa sand was measured in the lab under the Earth gravity (1g) using the Haines method (Rowell 1994). Dry Ottawa sand was first loosely poured into a Buchner funnel. The sample’s dry bulk density was 1.66 g/cm³, porosity was 0.37, and the sample height was 10 mm. Since the Ottawa sand is fairly uniform, it is assumed that the maximum possible porosity is 0.47 (at cubic packing) and the minimum possible porosity is 0.26 (at rhombohedral packing). The relative density (D_r) of the Ottawa sand used in the experiment is approximately 56%. After the sample was slowly saturated with water, suction was applied by lowering the burette at a 20 mm decrement. At each suction head, the volume of water drained from the sample was recorded. The drainage process continued until no water drained out upon further increasing the suction. Then the burette was raised to 20 mm increment to reduce the suction, and the volume of water that entered the soil sample under each suction head was recorded.

The rewetting process continued until the sample was saturated again. The experimental drying and rewetting curves were plotted in Fig. 7.

**Model Results and Discussion**

Fig. 7 shows the model results of water retention curves under rhombohedral and cubic packing of the Ottawa sand in zero gravity. Since the two extreme packing arrangements represent the most compact and the most porous pore structures, respectively, the two water retention curves represent the maximum range in variation that could result from possible particle rearrangement under zero gravity. The volumetric water content is a ratio of the volume of CEVSs that are occupied by pore fluid to the total bulk volume of the pore network. The results reveal that the bubbling suction—the pressure at which water starts to drain from a saturated porous medium—is much lower under cubic packing (about 100 mm) than under rhombohedral packing (about 280 mm).

Pore sizes are larger in cubic packing than in rhombohedral packing (Fig. 6), thus capillary pressure is lower and pore fluid drains more easily. The simulations show that the simulated water retention curves in 0g under both particle packing have sharp decrease immediately following the bubbling pressure, while the experimental drying curve in 1g has a gradual decrease in water content. The sharp decrease in water content might be due to the “piston flow” and uniform void ratio assumed in the model development. In reality, pore dimensions may be more various than presented in Fig. 6 and pore water may not vacate the pore entirely at a certain suction due to sorption and residual water held at corners of angular pores. In Fig. 7, the wiggle in the drying curve of the rhombohedral packing is due to the discontinuity of pore-throat distribution (Fig. 6) that was fed into the network model. The drying curve indicates that at the suction head of 280 and 300 mm, the volumetric water content is the same. Using Eq. (7), the pore throats corresponding to the capillary pressure head of 280 and 300 mm are 75 and 70μ, respectively. In Fig. 6, the pore throats of 75μ are not present in the pore-throat distribution for the rhombohedral packing. The smoothness of the WRC curves can be improved by adding more data points in the pore-throat distribution.

Fig. 7 also reveals the soil-water retention hysteresis. The hysteresis may be quantified by the difference or the ratio of the matric potential between the drying and rewetting curves at the same water content. In Fig. 7, the matric potential difference is 80–120 mm for cubic packing and 220–260 mm for rhombohedral packing, and the matric potential ratio is 4–5 for cubic packing and 4.5–6.5 for rhombohedral packing. Therefore, the model simulations reveal accentuated hysteresis when particle arrangement changed from loose condition (cubic packing) to compact condition (rhombohedral packing). Since the contact angles used in the two packing conditions are kept constant, the increased hysteresis is due to capillary hysteresis only. Jones and Or (1999) evaluated several data sets of water retention characteristics using spaceflight experiments (Morrow et al. 1994; Bingham et al. 1996) and also noticed that hysteresis in porous substrate was accentuated in microgravity. A recent study by Heinse et al. (2007) reported the water retention characteristics measured onboard the NASA’s KC135 microgravity flights, and the results show the wetting and drainage curves generally shifted to the lower matric potential. Fig. 7 shows that with the water retention curves shifting to lower matric potential under cubic packing, it can be deduced that microgravity is more likely to result in the cubic packing of particles. This is in agreement with the particle
separation under microgravity reported by Reddi et al. (2005).

Particle rearrangement could happen during the drying or rewetting process, resulting in a “dynamic” pore-size distribution and temporal change of water retention characteristics. This model studies the changes in water retention characteristics of the Ottawa sand during the drying process due to particle rearrangement from cubic to rhombohedral packing. The Ottawa sand sample is initially saturated under cubic packing. At suction head of 100 mm and volumetric water content of 0.46 during the drying process, the particle arrangement changes to rhombohedral packing. Due to the shrinkage of pores, pore water may be squeezed out into neighboring pores, and some pore water may drain out of the pore network from the bottom. After the particle rearrangement, the drying process continued under the new rhombohedral packing. The simulation results in Fig. 8 show that after the particle rearrangement the drying curve follows the drying curve of the originally rhombohedral packing. If the particle rearrangement (from cubic to rhombohedral packing) occurs at suction head of 140 mm when the volumetric water content (0.03) was close to residual water content, the drying curve changes little and it continues to follow the water retention curve under the cubic packing. The simulations indicate that water retention characteristics are less affected by the particle rearrangement at low water content than at high water content.

Fig. 9 depicts the pore-water spatial distributions when the particle arrangement changes from cubic packing to rhombohedral packing at a suction head of 140 mm during the drying process. The network dimension uses $10 \times 10 \times 5$ to obtain a better graphical presentation. The CEVSs occupied by water are presented in black color. Fig. 9(a) shows the spatial distribution of pore fluid in the pore network under cubic packing, in which 36 CEVSs are occupied by water. Fig. 9(b) shows the spatial distribution of pore fluid in the same sample under rhombohedral packing after the particle rearrangement at the same suction, and 52 CEVSs are occupied by water. The modeling results show that more pores are occupied by water due to the pore shrinkage, although the water content and saturation only increased slightly in this particular case (refer to the captions of Fig. 9) before and after the particle rearrangement. Fig. 9 also suggests that the pore fluid is not uniformly distributed in the porous medium. The model results are in agreement with the study by Podolsky and Mashinsky (1994) who observed local overmoistening in a substrate sample aboard the “Salyut-7” and “Mir” space stations.

Baked ceramic aggregates were previously used as a plant growth medium in spaceflight. The findings that are based on the Ottawa sand may be extended to the baked ceramic aggregates. Although the particle size distributions of the two materials are similar (Fig. 5), the water retention drying curves are quite different (Fig. 10). The major reason is that the baked ceramic aggregates have many micro pores (intra-aggregate pores), which hold water and do not easily give it up. Only the water in the macro pores (interaggregate pores) drains. This explains why the residual water content for this material is quite high (about 0.34). On the other hand, the macro pore structures of the two materials are similar due to the similar particle size distributions. If the water retention curve of the Ottawa sand is shifted vertically by the amount of the residual water content of the baked ceramic aggregates, the two curves become similar. Since the water easily available to root zone is in the macro pores, the findings based on the Ottawa sand in this paper can apply to the baked ceramic aggregates.
aggregates, if the residual water content of the baked ceramic aggregates is known.

Conclusions

This paper presents the variation of water retention characteristics due to particle rearrangement and the pore fluid spatial distribution in porous media under zero gravity. The 3D pore network model takes into account pore interconnectivity and pore nonuniformity. The pore-throat distributions used in the model are derived from particle size distribution with consideration of particle arrangement. The model results appropriately reflect the quantitative variation in the range of water retention curves due to possible particle rearrangement under zero gravity. The model simulations indicate increased hysteresis when particle arrangement changes from a loose to compact condition. Particle rearrangement (from cubic to rhombohedral packing) significantly alters the water retention characteristics when the porous medium is nearly saturated. When the porous medium is close to residual saturation, water retention characteristics are almost unaffected by particle rearrangement. Pore fluid spatial distribution in the porous media (Ottawa sands) is found to be nonuniform.

The model has the following limitations that need improvement. The model simulates piston flow and assumes that pore water vacates each pore entirely; and it does not consider water adsorption and absorption as well as the water retained at the corners of angular pores. The model assumes that all pores shrink during the vibration-induced compaction; it does not consider the possible localized pore dilation during compaction. The model does not simulate the actual pore variation under the combined effects of vibration and microgravity. The pore space of a loosely packed porous medium tends to shrink under vibration (Xiao et al. 2006), while under microgravity particles may separate and the pore structure dilates (Reddi et al. 2005). Under the combined effects of vibration and microgravity, particles rearrange so that pore body may reduce to pore throat, and pore throat may enlarge to pore body, making the realistic modeling of pore structure difficult. Further pore-scale experimental study of the pore variation under intermediate packing is needed so that a more realistic modeling of soil-water characteristics can be developed.

Acknowledgments

This research was funded by the Advanced Life Support Program of NASA Johnson Space Center (Project No. NAG9-1399). The support from this agency is gratefully acknowledged. The writers also thank the editor and the three anonymous reviewers for their helpful comments in improving the quality of this manuscript.

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