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A Micromechanical Study of Unsaturated Granular Material
Using DEM Simulation and X-ray CT

By: **Guohan Zeng**

University of Nottingham

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Abstract

In unsaturated soil, capillary bridges develop at the air-water interface within the pore space due to the cohesion deficiency on the side of the air phase. The interaction between capillary bridges and the soil particles make the mechanics of unsaturated soil complicated. Using the discrete element method (DEM), the behaviour of unsaturated granular materials can be predicted by including local interactions in numerical simulations. Many recent studies have been carried out to investigate the global soil properties with water-induced stresses homogeneously distributed in a granular medium. However, the quantity and spatial distribution of capillary bridges, which depends on the anisotropy and packing density of the particle arrangement, have not been well investigated. To better understand the mechanical properties of unsaturated soils, triaxial test simulations were carried out using particle assemblies with different matric suctions, varied water distribution models and various confining stresses.

Numerical testing simulation of dry triaxial tests was firstly used for calibration of the micro-mechanics of the numerical granular medium. Toroidal approximations for capillary bridges (between solid particles) were then adopted in the DEM simulations using the iterative method for estimating the geometries of the menisci. A series of water distribution models were presented for numerical specimens with different volume fractions that were permissible for capillary bridge formation. By conducting the triaxial test simulations, almost identical stress-strain behavior was observed for all distribution models with the same magnitude of liquid volume fraction. Higher stress ratios and increased

dilatancy could also be achieved using specimens with a larger liquid volume fraction. Moreover, the results showed that higher shear strength and larger deformation appeared to be generated in an unsaturated granular medium when the same amount of water was more widely distributed.

To validate the geometric information for the capillary bridges in the numerical model, X-ray CT was conducted using three unsaturated sample specimens consisting of spherical glass beads. Statistical image analysis was carried out using Avizo Fire v8.1 software. The merging of capillary bridges with liquid clusters leading to the formation of larger liquid ganglia, was observed when the saturation degree reached a critical limit. Capillary bridges with non-constant curvatures could develop between two solid particles without locating symmetrically to the axis passing through the particles' centroids. These observations also appeared to show the development of liquid rings at the particle-particle interface due to the prominent interface area.

The microscopic studies conducted here suggested that the strength of an unsaturated material could be significantly influenced by the coordination numbers of both water and (granular) solid. It was observed that the matric suction could dominate the water contact coordination number when the liquid phase was uniformly distributed. In this case, the ratio of coordination numbers between water and solid may thus be used as an efficient indicator for shear strength. The results also showed that the water contact coordination number appeared to be strongly dependent on the magnitude of liquid volume fraction.

When the saturation degree is constant, the larger coordination number ratio may also imply a wider distribution of capillary effects.

Keyword: DEM, X-ray CT, unsaturated granular material, capillary effect, water distribution, micromechanics

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Nomenclature

Symbols

α	Empirical parameter for describing SWCC	$\bar{\sigma}_{ij}$	Mean stress tensor
β	Angle of interparticle friction	σ_{ij}^{cap}	Capillary stress tensor
χ	Empirical factor referring to soil suction	σ_{ij}^d	Dimensionless stress tensor
δ	Hall-filling angle on particle	$\overline{\sigma}_{ij}$	Generalized expression of stress tensor under uniform stress state
δ_n	Particle overlap	ε_l	Axial strain
θ	Water content	ε_v	Volumetric strain
θ_r	Residual water content	ε_i^p	Plastic strain
θ_s	Saturated water content	ε_{vp}^p	Plastic volumetric strain in BBM
ϑ	Diffusion flux	ε_s^p	Plastic deviatoric strain in BBM
Ψ	Total suction	$\overline{\varepsilon}_{ij}$	Microstructural expression of strain tensor
ϕ	Solute concentration	ρ_d	Particle density
τ	Shear strength	ρ_w	Density of water
σ'	Effective stress	φ	Angle of contact direction
σ_1	Major principal stress	φ'	Effective angle of internal friction
σ_2, σ_3	Minor principal stress	ω_r	rotation of particle
σ_{ij}	Stress tensor	$\dot{\omega}_r$	Relative rolling angular velocity

ω_s	Solid contact coordination number	$D_{rupture}$	Rupture distance
ω_w	Water contact coordination number	e_r	Coefficient of restitution
ω_{wb}	Capillary bridge breaking number	e	Void ratio
μ	Friction coefficient	E	Yong's modulus
μ_r	Coefficient of rolling resistance	E^*	Effective Yong's modulus
η	Stress ratio	f_{cap}	Mean capillary force
η_r	Rolling viscous damping ratio	f_{cont}	Mean solid contact force
Δt	Time-step	f	Parameter of viscous damping torque
c'	Apparent cohesion for soils	F_{cap}	Capillary force
c_n	Normal damping coefficient of particle	F_{cont}	Contact force on particle
c_t	Tangential damping coefficient of particle	F_C	Mean contact force over all contact points
C_c, C_u	Coefficients for defining PSD	F^d	Dimensionless contact force
C_r	Damping constant	F_n	Normal force
C_r^{crit}	Rolling critical viscous damping constant	F_t	Tangential force
D	Interparticle distance	F_{UB}	Mean unbalanced force
D_E	Euclidian dimension	i	Number of iterations
D_F	Fractal dimension	I_r	Equivalent moment of inertia
D_o	Diffusion coefficient	k	Increasing slope of cohesion

k_n	Particle normal stiffness	r_{ext}	External radius of capillary bridge
k_r	Rolling stiffness	R	Particle radius
k_t	Particle tangential stiffness	R_r	Rolling radius
m	Mass of particle	R_s	Curvature of the contractile skin
M	Slope of the critical state line	$\bar{R}$	Mean particle radius
M_r	Rolling resistance torque	S	Matric suction
M_r^d	Rolling viscous damping torque	S'	Area of contact surface
M_r^m	Limiting spring torque	S^*	Dimensionless form of matric suction
M_r^k	Spring torque	Sr	Degree of saturation
n	Porosity	Sr_e	Effective saturation degree
n_j^c	Dimension less form of internal fabric	Sr_r	Residual saturation degree
N	Number of particles	Sr_t	Target saturation degree in experimental observation
p	Mean total stress	t_j^c	Dimension less form of internal fabric
p'	Mean effective stress	T	Water surface tension
p^c	Reference stress state	T_s	Surface tension
p'_0	Isotropic yield stress	u_a	Air pressure
$\bar{p}$	Mean net stress	u^c	Friction Mechanism
q	Deviatoric stress	U_s	Sliding component of rolling resistance model

r_{int}	Internal radius of capillary bridge	U_r	Rolling component of rolling resistance model
V	Volume of particle assembly	Abbreviations	
V_a	Total volume of pore space	BBM	Barcelona Basic Model
V_{cap}	Volume of capillary bridge	CSL	Critical State Line
V_s	Total volume of glass beads in the test tube	DEM	Discrete Element Method
V_t	Volume of test tube	MCC	Modified Cam Clay Model
W_θ	Weight of imposed water in experimental specimen	NCL	Normal Consolidation Line
W_s	Total weight of glass beads in the test tube	PSD	Particle Size Distribution
W_w	Weight of test tube with caps	RVE	Representative Elementary Volume
W_{w1}	Total weight of test tube with caps, glass beads and water	SWCC	Soil Water Characteristic Curve
x_{c1}	locations of the ends of meniscus	XRCT	X-ray Computed Tomography
y_0	neck radius of capillary bridge		
$y(x)$	profile of capillary bridge along the x axis		
$\{\sigma'\}$	Stress state		
$\{k\},\{m\}$	State parameter for the Cam Clay Model		

CHAPTER 1: Introduction

1.1 Background

Unsaturated soil formation strongly depends on the local microclimate ([Fredlund and Rahardjo, 1993](#)). Both evaporation and precipitation can change the water content in soils. Most of the soil deposits of sands, silts and gravels above the water table are found as partially saturated ([Smith, 1998](#)). In a simplified form, unsaturated soil contains three phases: soil particles, water and air. The interactions and the variety of their physical and chemical properties make the mechanics of unsaturated soil more complicated than others. Capillary bridges develop at the air-water interface due to the cohesion deficiency on the side of the air phase. Resulting from the surface tension from the contractile skin, capillary force depending on the water content is introduced acting between soil particles. Moreover, granular materials are usually composed of distinct particles with specific interparticle interactions that are influential on their macroscopic behaviour. Particle scale modelling therefore becomes a pertinent approach for unsaturated granular soil mechanics correlating physical fundamentals to locally induced effects.

Since both capillary pressure and soil shear strength are strongly related to the degree of saturation, it is rational to establish a constitutive function of the water content directly involving capillary effects. Many recent studies and experiments have been carried out to investigate global soil properties with water-induced stresses homogeneously distributed in the medium ([Scholtès *et al.*, 2009](#)). For a

pendular regime with disconnected water phase, applying capillary theory can relate the forces induced by the capillary bridges to the local geometry of the particles and the capillary pressure. However, the quantity and spatial distribution of capillary bridges have not been well investigated. New techniques such as X-ray computed tomography (X-ray CT) allows researchers to obtain 3D information at mesoscale, and thus achieve characterization of unsaturated soil microstructure ([Bruchon, 2013](#)). To further study and better interpret unsaturated soil, both numerical modelling and experimental observations will be presented in the project.

By the discrete element method (DEM), the behaviour of unsaturated granular materials can be predicted by including local interactions in numerical simulations. DEM was initially developed to simulate the behavior of dry granular materials according to the direct relations between external loads and the interparticle forces ([Cundall and Strack, 1979](#)). Due to the agreement between experimental observations and DEM simulations, it has recently become a popular tool and evolved into a mature technique for unsaturated granular materials. Many studies have been carried out using DEM with uniform water distribution, dealing with capillary effects for grains with equivalent diameters ([Farouk, 2004](#)). However, a real soil assembly usually contains water phase with a random distribution due to different activities such as precipitation. As the capillary force can be highly dependent on the particle diameter, it is also necessary to consider the effect of particle size when investigating the origin of capillary strength. By modelling monodisperse packings incorporating well-defined rules of water distribution and the elementary laws under an external

load, macroscopic behaviour and stress-strain relationships of unsaturated soil can be more accurately simulated along a set of increasing water contents.

1.2 Project Aim and Objectives

The main aim of this project is to propose a modified 3-dimensional numerical DEM model that enables interpretation of mechanical behavior, with variable water distribution, in unsaturated granular soils with low saturation degree. To demonstrate the modelling results, experiments using X-ray CT are conducted for observations of the amount and spatial distribution of capillary bridges at low water content. Investigation of the origin of capillary strength is presented by carrying out microscopic analyses. The major objectives of this research are to:

- Determine the influence of the spatial distribution of capillary bridges on the triaxial stress state in unsaturated soils in the pendular regime.
- Validate the numerical model predictions against experimental data for dry granular soils.
- Quantify the relationship between the saturation degree and the coordination number of capillary bridges.
- Microscopic characterization of the critical state of unsaturated granular material.
- Determine the influence of particle size in a monodisperse material on the capillary strengthening effect.
- Investigate the origin of capillary strengthening effect in unsaturated soil.
- By altering the capillary bridge distribution in an unsaturated soil to increase its

strength in a triaxial test.

1.3 Thesis Outline

The research background and the objectives of this study are presented in **chapter 1**, with the thesis outline.

Chapter 2 is a general literature review for this study. The major findings in unsaturated soil mechanics are summarized. The achievements of DEM and the developments of granular material micromechanics are introduced. The image processing techniques commonly adopted are also presented.

The numerical techniques implemented in this study are demonstrated in **chapter 3**. The capillary bridge model, the suction controlled triaxial test method in DEM simulations are introduced. The preparation procedures of the experimental specimens and the processing methods for the digital images are also presented.

Chapter 4 firstly presents a numerical assembly of Leighton Buzzard (LB) sand fraction E to reproduce the mechanical behaviour of dry granulates under triaxial compression at the macroscopic scale. Rolling resistance was adopted between contacting particles for dry assemblies. Suction controlled triaxial test simulations were then conducted using spherical particles with capillary bridge geometries estimated by the toroidal approximation. Distribution models for capillary bridges are later introduced to investigate the influence of their spatial distribution. The macroscopic behaviour of various distribution models under

triaxial compression tests is also presented. Eventually, simplified water distribution models are introduced to represent random water distribution with the same liquid volume fraction. The effect of particle size on the capillary effect was also investigated using the simplified distribution models.

Experimental observations conducted by X-ray CT are presented in **chapter 5**. To further understand the interplay between the mechanical properties and the water content in unsaturated materials, investigations of the geometric information and spatial distribution of capillary bridges are carried out using image processing. Three phases (air, water and particle) were segmented using the thresholding technique. Porosity and saturation degree were determined for each unsaturated specimen. Particles are separated using the watershed algorithm, and the particle size distribution curve is also plotted for each specimen. The number of liquid clusters is determined by applying a series of filters to the binary image of the water phase. Size distribution of liquid clusters is also estimated by labelling the disconnected objects and calculating their individual volume. Investigation of the local geometric information of a capillary bridge is later carried out by comparing the observations with the analytical solutions. The spatial distribution of water is also translated using a cubic model, specifying the local saturation degrees in specific regions.

A preliminary study of the critical state of unsaturated materials is firstly presented in **chapter 6**. Numerical specimens with uniform capillary effects were adopted, and the triaxial shearing was applied to both loose and dense specimens at different stress levels with various suctions. With the

implementation of different distribution models, the study of liquid distribution at particle scale is presented later. The relationship between material strength and various microscopic parameters, including contact coordination numbers and interparticle forces are investigated. The roles of coordination numbers, matric suction, saturation degree and the magnitude of liquid volume fraction are analysed and discussed. Using the simplified distribution model, the origin of strength is investigated and related to the coordination number ratio. The increased capillary strengthening effect, developed by specimens with smaller particle size, is also analysed at particle scale.

In **chapter 7**, the major conclusions of this study are summarized. Suggestions for the future study of unsaturated soils are presented.

CHAPTER 2: Background

2.1 Unsaturated Soil

2.1.1 Introduction

The microclimatic condition within an area is the most critical factor that leads the soil deposit to become unsaturated (Fredlund and Rahardjo, 1993). Rainfall, as the main source of subsurface water could penetrate downwards and consequently fill up the voids in soils. Both evaporation from plants and the soil surface and the transpiration from the vegetative cover can lead to water reduction in soils. Subsurface water can be divided into two zones: aeration zone and saturation zone (Figure 2.1.1.1).

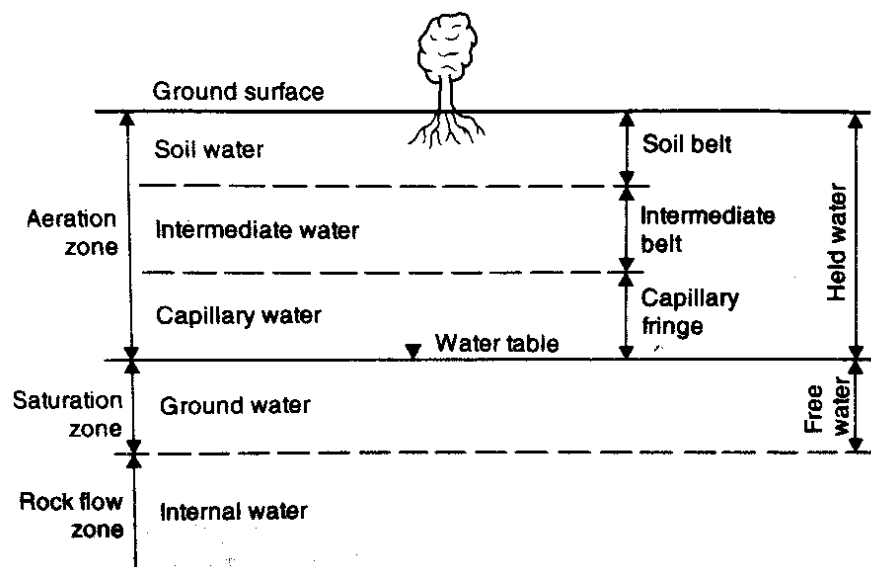


Figure 2.1.1.1 Illustration of subsurface water (Smith, 1998).

The aeration zone occurs between the water table and the ground surface. In practical engineering problems, many of the deposits such as sands, silts, and gravels in this area are found unsaturated. Although clays are generally considered as saturated, they could become partially saturated in their upper

region (Smith, 1998). A soil assembly could contain up to three phases, which are liquid (water), gas (air) and solid (soil particle). The pressure of the pore-water in the soil is given the symbol u_w and the pressure of the air is given the symbol u_{air} . S_r stands for the degree of saturation, and is defined by:

$$S_r = \frac{\text{Volume of water } (V_w)}{\text{Volume of voids } (V_v)} \quad (2.1.1)$$

Saturated soil is considered to contain no air and its voids are full of liquid and in contrast, no liquid exists in a dry soil and gas completely fills its voids. When both liquid and gas exist in the voids of a soil the soil is defined as being partially saturated or unsaturated. Figure 2.1.1.2 shows a sample of unsaturated soil with continuous gaseous phase.

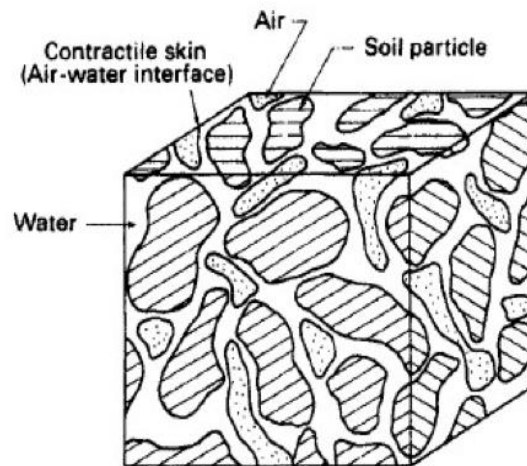


Figure 2.1.1.2 Unsaturated soil model with continuous gaseous phase (Fredlund and Rahardjo, 1993).

In geotechnical engineering practice, collapsing soils, residual soils and swelling clays are commonly regarded as problematic soils (Fredlund and Rahardjo, 1993). Due to the appearance of three phases, the interaction within and between them constitutes the mechanics of unsaturated soils which is much more complex than that of dry or saturated soils. Figure 2.1.1.3 shows the interparticle

forces generated by matric suction in an unsaturated soil sample ([Leshchinsky et al., 2010](#)).

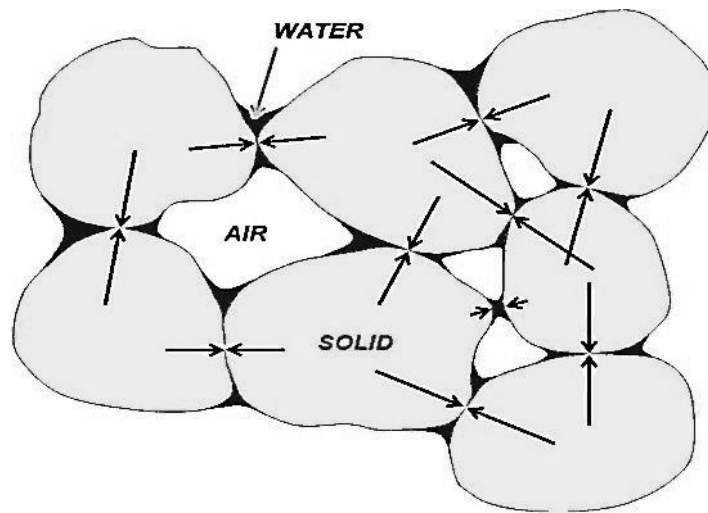


Figure 2.1.1.3 Interparticle forces generated by matric suction ([Leshchinsky et al., 2010](#)).

For an unsaturated soil system in equilibrium, external pressure can be balanced by the components of pressure and stress due to the phases and their interactions. These components can be given by the air pressure, water pressure, water vapour in air, dissolved air in water, meniscus formed at the water-air interface, interaction between soil particles and the pressure on a soil particle arising from the surrounding liquid. Since some of these pressures and stresses have very little effects at equilibrium, it is important to more thoroughly understand the influences of the interactions and phases to the overall soil behaviour ([Murray and Sivakumarv, 2010](#)).

2.1.2 Soil Suction

As described above, various forms of free water can filtrate from the surface down towards the water table and pass through soils whose permeability allows. This capacity of a soil to retain water within its own structure is considered as

soil suction. Soil suction is one of the major factors influencing the behaviour of unsaturated soil. Both matric and osmotic suction, although completely independent and having no effect on each other, can affect the total suction in a soil:

$$\Psi = s + \pi_o \quad (2.1.2)$$

where, Ψ stands for the total suction, s is the matric suction and π_o is the osmotic suction. Due to the appearance of capillary effects, matric suction varies with time while the environment changes and its variation could influence the overall equilibrium of the soil mass ([Fredlund and Rahardjo, 1993](#)). It is one of the critical factors that influences unsaturated soil mechanics. In unsaturated soils, it is generally accepted that the value difference between air pressure (u_a) and water pressure (u_w) at their interface is defined as matric suction (s), or capillary pressure. Therefore, matric suction can be commonly expressed by:

$$s = u_a - u_w \quad (2.1.3)$$

For many situations in geomechanics, air pressure (u_a) is usually atmospheric pressure. It can be taken as a datum and has a value of zero in most soil calculations ([Smith, 1998](#)). In this case, the matric suction value (s) is always positive since the water pressure (u_w) is normally negative for an unsaturated soil. A molecule in the interior of water experiences equal forces in all directions. However, a meniscus would appear at the air-water interface due to the deficiency of cohesive force on the side of air (Figure 2.1.2.1). In the soil voids, water molecules bond the air with the soil particles. Due to the pressure difference (s) between the two phases, a meniscus develops at the air-water

interface and there will be an additional surface tension (T_s) on the contractile skin that maintains the force equilibrium (Figure 2.1.2.2).

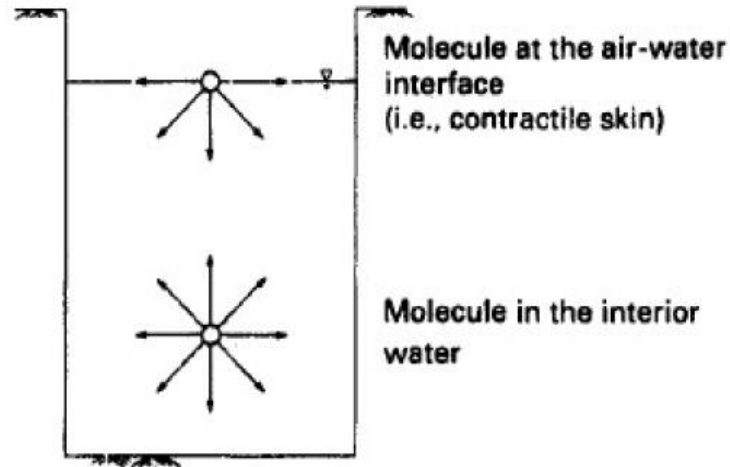


Figure 2.1.2.1 Intermolecular forces on contractile skin and in interior water (Fredlund and Rahardjo, 1993).

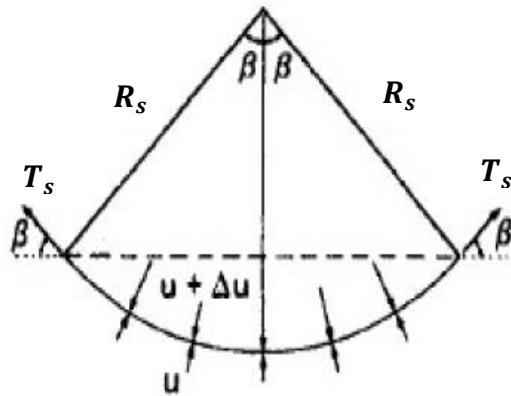


Figure 2.1.2.2 Pressures and surfaced tension acting on a curved 2D surface (Fredlund and Rahardjo, 1993).

For the assumption of equivalent curvatures, the capillary pressure on the contractile skin can be related to the surface tension (T_s) and the curvature (R_s):

$$s = u_a - u_w = \frac{2T_s}{R_s} \quad (2.1.4)$$

This equation is known as the Young-Laplace equation. For menisci with different curvatures R_1 and R_2 , it is expressed as:

$$s = u_a - u_w = \frac{T_s}{R_1 + R_2} \quad (2.1.5)$$

Smith (1998) also revealed that the matric suction value in an unsaturated soil varies over the whole range of the possible water content. The value of matric suction starts as zero when a soil is saturated, and it increases to a peak while the water content decreases to be completely dry. During the decrease, the air breaks through at a given state. The value of matric suction at that point is defined as the air-entry pressure which significantly depends on pore size. The soil sample afterwards becomes unsaturated. Due to the interface actions between water and air, capillary forces start to increase. The state where pore water is interconnected, and air exits in bubble form is defined as the capillary regime. In the funicular regime, both pore water and air phase are interconnected. The pendular regime of a soil is reached when the water phase becomes discontinuous. In a pendular regime, the capillary effect forms a bond known as a capillary bridge between soil particles providing an interparticle cohesive force (Fredlund and Rahardjo, 1993). Figure 2.1.2.3 demonstrates the schematic presentation of different saturation regimes (Mitarai and Nori, 2006).

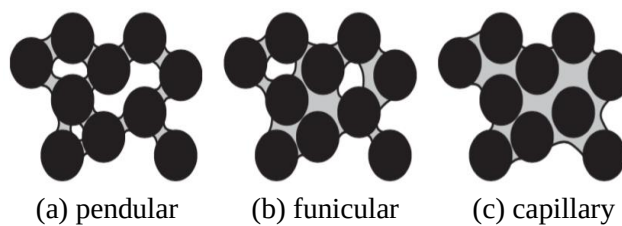


Figure 2.1.2.3 Schematic presentation of different saturation regimes (Mitarai and Nori, 2006).

On the other hand, osmotic suction which is mainly related to the solute content in soil pore water could also lead to changes in the overall volume and shear strength of an unsaturated soil (Tindall and Kunkel, 1999). Although osmotic

suction is generally found to be relatively small when compared to matric suction for natural soil materials, it is still important to recognize its role in affecting unsaturated soil behaviour. Research has shown that the presence of salts within the soil water could lead to some fundamental changes in soil behaviour (Murray and Sivakumarv, 2010). Due to the difference in salt concentrations in the pore water of a soil assembly and surrounding water, osmotic suction could attract or remove water from the system. It represents the ion potential in the pore water and can be controlled by changing the water volume or the quantity of ions in the fluid (Fredlund and Rahardjo, 1993). Figure 2.1.2.4 demonstrates how osmotic suction attracts and releases water from a soil system (UoT, n.d.).

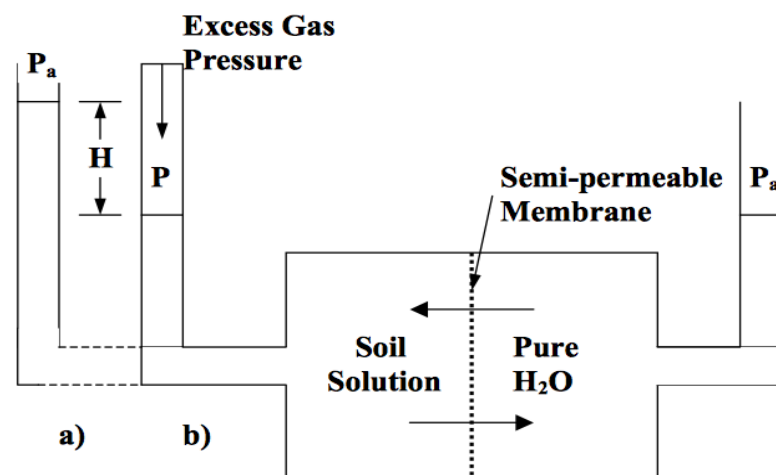


Figure 2.1.2.4 Interpretation of osmotic suction (UoT, n.d.).

This figure shows that water flows through the membrane into the solution due to the osmotic suction in the solution, and moreover due to the applied pressure on the solution, water flows into the pure water. Therefore, it can be deduced that the osmotic pressure of the solution equals the pressure on the solution required to balance the flow of fluid. According to Fick's first law, the diffusive flux goes from regions of higher concentration to regions of lower concentration

under the assumption of steady state, with a magnitude which is proportional to the concentration gradient. The required pressure can be derived in this way with certain a solute content:

$$\vartheta = -D \frac{\partial \phi}{\partial x} \quad (2.1.6)$$

where $\vartheta \left(\frac{mol}{m^2_s} \right)$ is the diffusion flux which is determined by the amount of substance flowing through a given area in a given time interval. $D_o \left(\frac{m^2}{s} \right)$ stands for the diffusion coefficient. $\phi \left(\frac{mol}{m^3} \right)$ is the solute concentration and $x \left(m \right)$ represents the position.

2.1.3 Pendular Capillary Bridge

Various research results have shown that in the pendular regime the capillary effect forms a bond between soil particles with an interparticle distance (D) due to the menisci at contractile skin (Fredlund and Rahardjo, 1993). This kind of bond could generate an attractive capillary force between the bonded particles, and is defined as a capillary bridge. They could develop between a pair of adjacent particles not necessarily in contact.

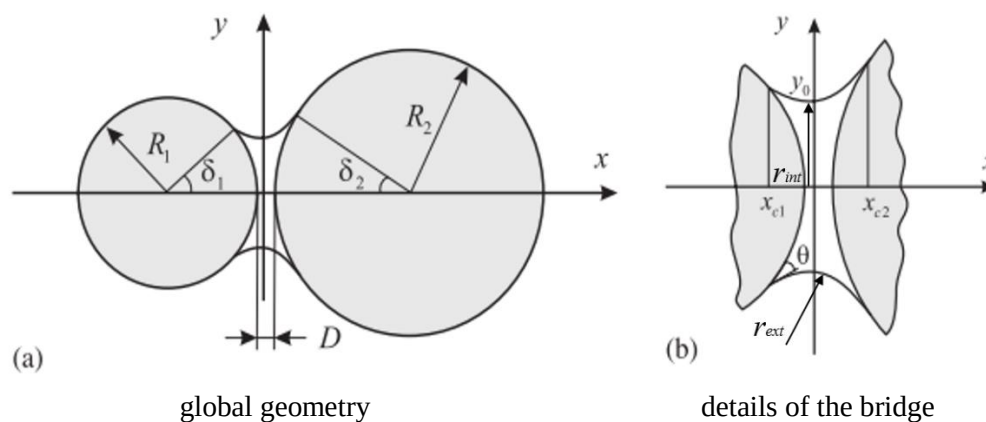


Figure 2.1.3.1 Capillary bridges between two particles of unequal sizes (Scholtes, 2009).

Figure 2.1.3.1 shows a capillary bridge developed between two spherical particles with different diameters. Developed by Soulié *et al.* (2006a), the internal (r_{int}) and external curvature (r_{ext}) of the capillary bridge can be expressed mathematically:

$$\frac{1}{r_{int}} = \frac{1}{y(x)\sqrt{1+y'^2(x)}} \quad (2.1.7)$$

$$\frac{1}{r_{ext}} = \frac{y''(x)}{(1+y'^2(x))^{3/2}} \quad (2.1.8)$$

The volume of the capillary bridge and the interparticle distance are given by:

$$V = \pi \int_{x_1}^{x_2} y^2(x) dx - \frac{1}{3}\pi R_1^3(1 - \cos\delta_1)^2(2 + \cos\delta_1) - \frac{1}{3}\pi R_2^3(1 - \cos\delta_2)^2(2 + \cos\delta_2) \quad (2.1.9)$$

$$D = R_2(1 - \cos\delta_2) + x_{c1} + R_1(1 - \cos\delta_1) - x_{c2} \quad (2.1.10)$$

where δ_1 and δ_2 are the filling angles for two particles. x_{c1} and x_{c2} refer to the locations of the ends of the meniscus. R_1 and R_2 stand for the particle radii and D is the interparticle distance. The capillary bridge between two spherical smooth particles of unequal diameters can therefore be described by the Laplace-Young equation:

$$\frac{s}{T_s} (1 + y'^2(x))^{\frac{3}{2}} + \frac{1 + y'^2(x)}{y(x)} - y''(x) = 0 \quad (2.1.11)$$

where $y(x)$ is the profile of the capillary bridge along the x axis which is the liquid-air interface. Different methods have been presented for the determination of the resultant force in this case. The gorge method is suggested in many studies, for example, Lian *et al.* (1993) and Soulié (2006a). By this method, the capillary

force resulting from the presence of the capillary bridge is calculated at the gorge, using the neck radius (y_0):

$$F_{cap} = 2\pi y_0 T_s + \pi y_0^2 s \quad (2.1.12)$$

Based on the assumption of a parabolic or toroidal shape, the capillary forces are generally derived according to the geometrical characteristics of the capillary bridge, such as its filling angle, diameter and the internal and external curvature (Fairbrother and Simons, 1998). Nevertheless, it is difficult to accurately measure these parameters. Most expressions do not involve the evolution of capillary force with the force-displacement relationship accounting for the degree of saturation as a macroscopic quantity.

2.1.4 Soil Water Characteristic Curve

The soil water characteristic curve (SWCC), also called soil water retention curve (SWRC) can be used to define the ability of unsaturated soil to attract water at various water contents and suctions (Fattah, 2013). Thus, it could help to study the water distribution and the relation between soil suction and water content in granular media.

It is agreed that SWCC relates the water content of a soil to its matric suction and is a significant hydraulic property related to the size and connectivity of the soil microstructure. The SWCC is distinct to each type of soil material. Since it is strongly dependent on the soil texture and microstructure, it can help to better understand the water distribution in partially saturated soil materials. Figure 2.1.4.1 presents typical soil water characteristic curves for different soil textures. At a given matric suction, the SWCC can indicate the amount of water retained

in a soil mass under equilibrium. As a generic feature of unsaturated soil materials, the polydisperse particle system could directly lead to different characteristics of pore structure. Researchers have found that the macroscopic cohesion of an unsaturated granular material increases when a wider distribution of particle sizes are adopted. (Voivret *et al.*, 2009). It was also suggested that the air entry value and the slope of SWCC could depend on the particle size distribution (Yang *et al.*, 2004).

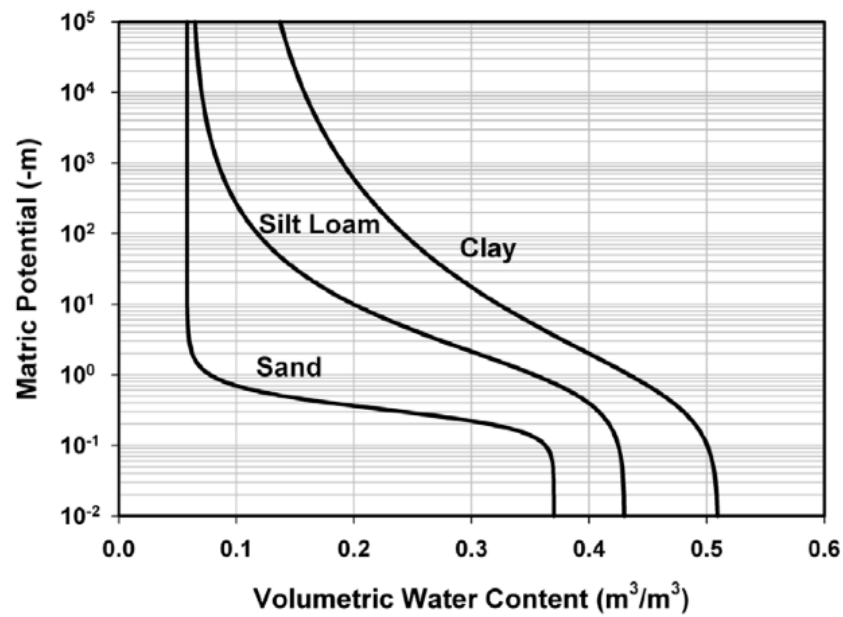


Figure 2.1.4.1 Typical soil water characteristic curves for different soil textures (Tuller and Or, 2003).

The characterization and estimation of the SWCC has been a key focus of geomechanical research in the recent decades. Van Genuchten (1980) suggested an empirical parametric model for describing SWCC:

$$Sr_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{(1 + (\alpha s)^n)^{1-\frac{1}{n}}} \quad (2.1.13)$$

where Sr_e is defined as the effective saturation degree, ϕ is to the matric suction, θ is the water content, and θ_s and θ_r stand for the residual water content and saturated water content respectively, α and n are both empirical parameters.

Moreover, using fractal distribution of pore structure can provide a more realistic model of pore-water distribution. Tyler and Wheatcraft (1990) firstly provided a model based on fractal theory to predict the SWCC:

$$\frac{\theta}{\theta_s} = \left(\frac{\varphi}{\varphi_{min}}\right)^{D_F - D_E} \quad (2.1.14)$$

where φ_{min} is the air entry value of matric suction. D_E is the Euclidian dimension, equal to 2 or 3 for 2-dimendional or 3-dimensional systems. The fractal pore water distribution in this model is assumed to be a Sierpinski carpet. D_F is the fractal dimension of the SWCC, and therefore can be expressed by:

$$D_F = \frac{\log((b^i)^{D_E} - n)}{\log(b^i)} \quad (2.1.15)$$

where b is a scaling factor, n is the number of squares or cubes removed at every iteration and i is the number of iterations. This model with fractal pore-water distribution based on the power-law form of the SWCC (Brookes and Corey, 1964; Campbell, 1974) was later proved to be a pore-solid fractal model with limitations (Rieu and Sposito, 1991). Rieu and Sposito also suggested the mass fractal dimension as the most sensitive parameter. Numerous research studies haven been carried out since then and different models have been presented. Perfect (1999) presented a new model:

$$\frac{\theta}{\theta_s} = \frac{(\varphi)^{D_m - 3} - (\varphi_{max})^{D_m - 3}}{(\varphi_{min})^{D_m - 3} - (\varphi_{max})^{D_m - 3}} \quad (2.1.16)$$

where φ_{max} stands for the matric suction value when the largest pore space is developed. D_m is the mass fractal dimension. Research has shown that this model could approximately cover the entire soil water retention data from over

dryness to saturation ([Ghanbarian-Alavijeh et al., 2011](#)). However, it is difficult to efficiently determine the value of φ_{max} .

2.1.5 Shear Strength

To predict the stability of the soil mass, it is essential to estimate its shear strength. For saturated soil materials, the Mohr–Coulomb theory introduced by Terzaghi ([1936](#)) has been successfully used to predict the shear strength in practice for decades. However, unsaturated granular soils present a complicated nonlinear response resulting from interactions between soil particles. These interactions depend greatly on different factors, such as soil texture, soil skeleton, particle size distribution, water distribution, capillary force and the surface tension across the contractile skin. Recent investigations have shown that shear strength models of unsaturated soils can be correlated with the soil water characteristic curve, which might be further related to particle size distribution ([Fredlund and Vanapalli, 2002](#); [Jiang, 2004](#)). In a pendular regime, experimental results indicate that the shear strength of the soil can be significantly influenced by the capillary-induced tensile stress and the hysteresis ([Richefeu, 2006](#); [El Shamy and Gröger, 2008](#)).

Different forms of correlation have been proposed for the tensile strength of unsaturated granular materials. Bishop ([1959](#)) firstly introduced the idea of effective stress:

$$\sigma' = (\sigma - u_a) + \chi(u_a - u_w) \quad (2.1.17)$$

where σ' is the effective stress, u_a and u_w are pore water and pore air pressure. χ is an empirical factor referring to soil suction. $(\sigma - u_a)$ and $(u_a - u_w)$ are referred to as the net stress and matric suction respectively. In this case, the shear strength (τ) can be expressed using the Mohr-Coulomb failure criterion:

$$\tau = c' + [(\sigma - u_a) + \chi(u_a - u_w)]\tan\phi' \quad (2.1.18)$$

where c' defines the apparent cohesion for soils, and is zero for granular materials. ϕ' is the effective angle of internal friction. However, later research proved that Equation 2.1.17 has limitations when describing the deformation of unsaturated soils ([Jennings and Burland, 1962](#)). A reliable solution was proposed by using two independent stress-state variables to express the relation of an unsaturated soil ([Fredlund and Rahardjo, 1993](#)):

$$\tau = c' + (\sigma - u_a)\tan\phi' + (u_a - u_w)\tan\phi^b \quad (2.1.19)$$

where $\tan\phi^b$ represents the rate of increase in shear strength due to matric suction. Figure 2.1.5.1 illustrates the extended Mohr-Coulomb failure surface in a three-axis space. In the graph, the failure criterion for saturated soil can be recognized as a special case of that for unsaturated soil when $u_a - u_w = 0$, *i.e.* no matric suction exists.

Including the further physical explanations, Oberg and Sallfors ([1997](#)) proposed applying $\chi = Sr$ in their later study to describe a non-linear shear strength function:

$$\tau = c' + (\sigma - u_a)\tan\phi' + Sr(u_a - u_w)\tan\phi' \quad (2.1.20)$$

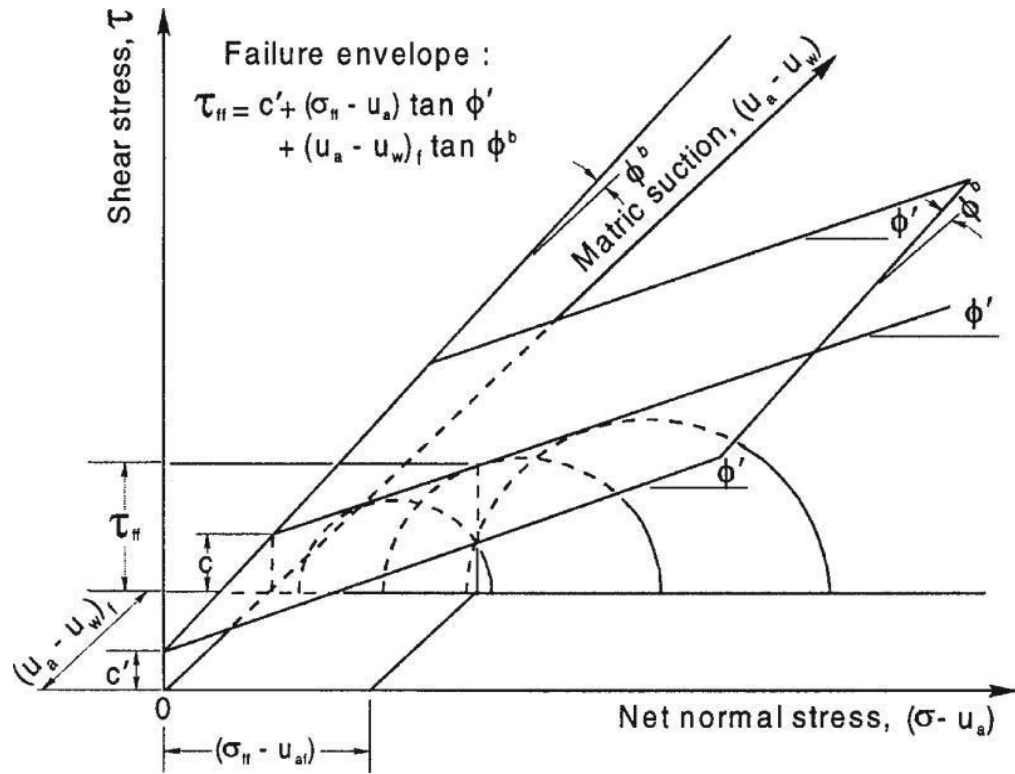


Figure 2.1.5.1 Extended Mohr-Coulomb failure surface for unsaturated soil
(Fredlund and Rahardjo, 1993).

Moreover, Vanapalli *et al.* (1996) considered the residual saturation degree ($Sr_{(r)}$) and thereby developed a new model based on Equation 2.1.20:

$$\tau = c' + (\sigma - u_a) \tan \phi' + \frac{Sr - Sr_{(r)}}{100 - Sr_{(r)}} (u_a - u_w) \tan \phi' \quad (2.1.21)$$

2.2 Constitutive Models

2.2.1 Critical State Model

The first critical state models were developed in 1963. It began as the original Cam Clay model and Modified Cam Clay model (Roscoe and Schofield, 1963; Schofield and Wroth, 1968). These critical state frameworks gave enough space of development of later constitutive models. Most constitutive models are elastoplastic with various components including a yield function, a plastic

potential function, a hardening/softening rule and yield surface elastic behavior definition. A yield function is expressed as:

$$F(\{\sigma'\}, \{k\}) = 0 \quad (2.2.1)$$

where $\{\sigma'\}$ is the stress state, $\{k\}$ are state parameters. This function represents those surfaces separating elastic from elastoplastic behaviour. Two functions for different Cam Clay models has been deduced as:

a) Cam Clay Model:

$$F(\{\sigma'\}, \{k\}) = q + Mp' \ln \left(\frac{p'}{p'_0} \right) = 0 \quad (2.2.2)$$

b) Modified Cam Clay Model:

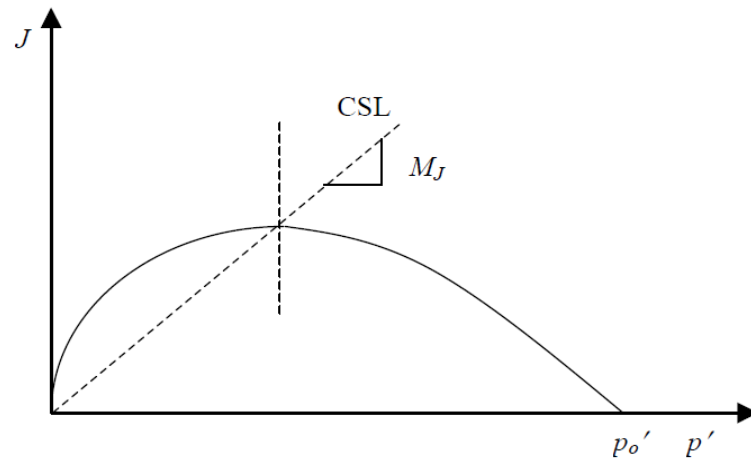
$$F(\{\sigma'\}, \{k\}) = \left(\frac{q}{p' M_f} \right)^2 - \left(\frac{p'_0}{p'} - 1 \right) = 0 \quad (2.2.3)$$

where p' expresses the mean effective stress, q is the deviatoric stress, M_f is defined as a model parameter, p'_0 is the isotropic yield stress. Figure 2.2.1.1 shows these yield surface projections.

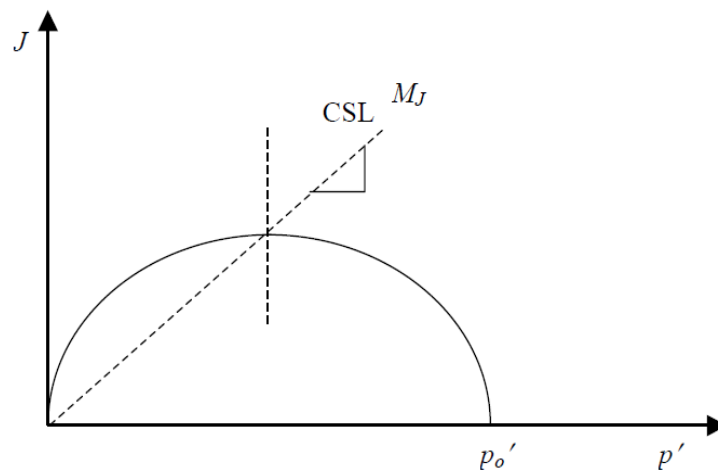
A plastic potential function can be expressed as:

$$P(\{\sigma'\}, \{m\}) = 0 \quad (2.2.4)$$

where $\{m\}$ are the state parameters. This function relates to the plastic strains on each point of the yield surface and the critical state line. It can determine relative magnitudes of plastic strains or the position of the critical state line in forms of different parameters, for instance, specific volume (v), mean effective stress (p') and deviatoric stress (q). Figure 2.2.1.2 gives its relation on the surface.



(a) Cam Clay



(b) Modified Cam Clay

Figure 2.2.1.1 Projection of yield surfaces (Roscoe and Burland, 1968).

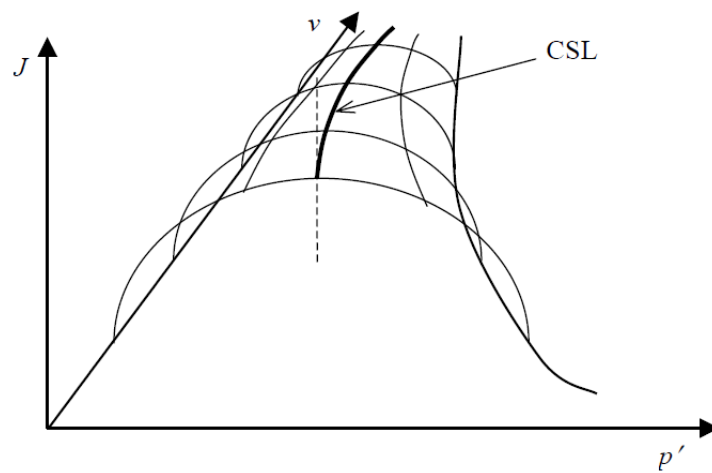


Figure 2.2.1.2 Boundary surface for modified Cam Clay (Roscoe and Burland, 1968).

From the figure above, it can be observed that the saturated soil yields at stress p_0^* , while the unsaturated soil yields at stress p_0 . The virgin compression line at constant value of suction can be expressed as:

$$v = N(s) - \lambda(s) \ln \frac{p}{p^c} \quad (2.2.7)$$

where p^c is the reference stress state at a relatively low stress level, $N(s)$ is the specific volume at $p_t = p^c$, $\lambda(s)$ is referred as the stiffness parameter related to suction. The isotropic unloading-reloading paths under constant suction are assumed to be elastic:

$$dv = -\kappa \frac{dp}{p} \quad (2.2.8)$$

where κ is defined as the parameter of the unloading-reloading path. When the deviatoric stress is applied to unsaturated soils, such as during triaxial loading, the elastic-plastic behaviour is then governed by the yield surface.

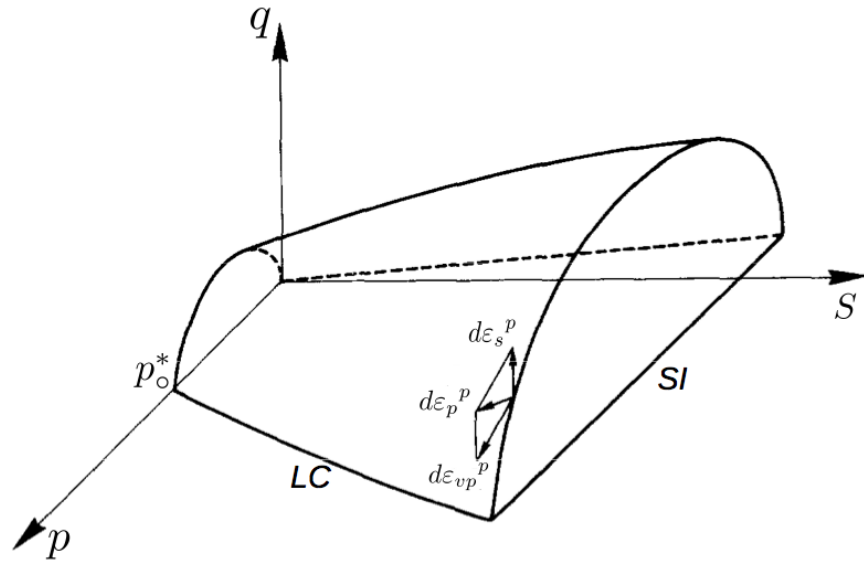


Figure 2.2.2.2 Yield surfaces of unsaturated soil in the (q, p, s) stress spaces (Alonso *et al.*, 1990).

The yield surface in BBM is formulated in (q, p, s) stress space, where q is referred to as the deviator stress, p is the net mean total stress and s is the soil suction (Figure 2.2.2.2).

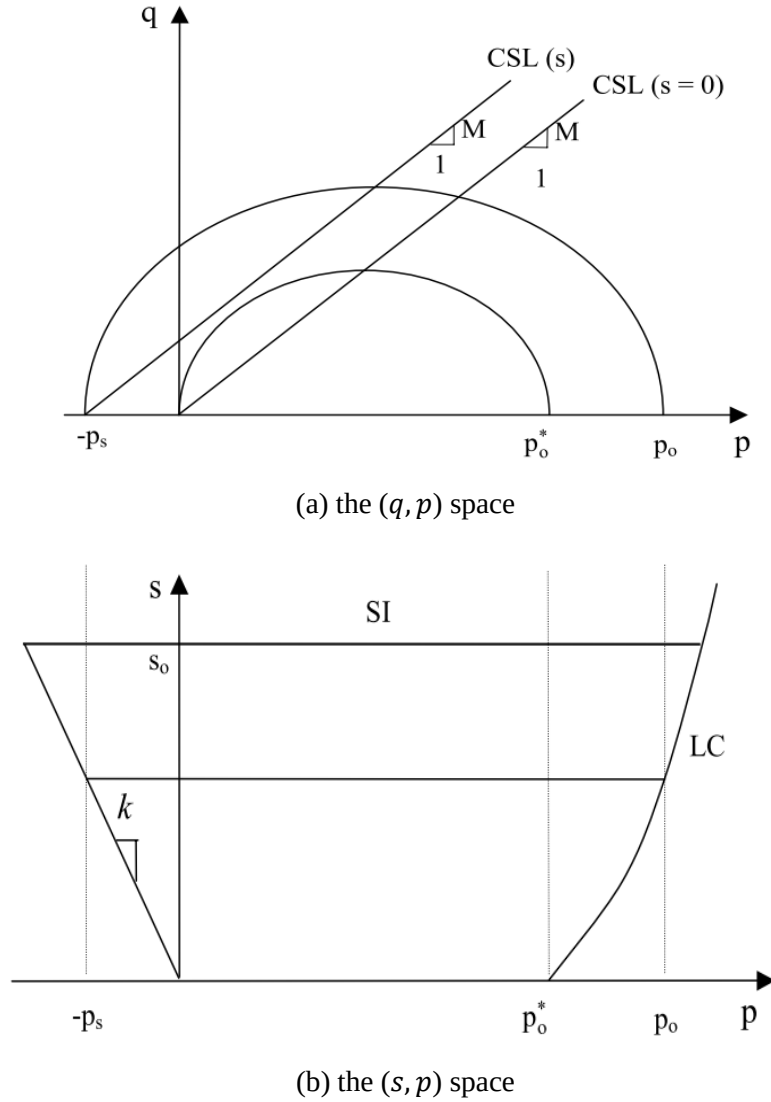


Figure 2.2.2.3 Yield surfaces of unsaturated soil in (q, p) space and (s, p) space (Alonso *et al.*, 1990).

Moreover, Figure 2.2.2.3 shows the yield surfaces in (q, p) space and (s, p) space (Alonso *et al.*, 1990). The boundary of the yield surface with different suctions is referred to as the Loading-Collapse (LC) curve (Figure 2.2.2.3b). The stress state within the LC curve is in the elastic domain. Under the wetting process which could lead to reduction in soil suction, collapse can happen to the

soil with the stress state developing along this curve. It can be observed from the yield surface that the BBM model obeys the MCC model when a soil is fully saturated (*i.e.* no suction). When the suction increases, the size of the elastic domain enlarges.

The yield surfaces are expressed by:

$$q^2 - M^2(p + p_s)(p_0 - p) = 0 \quad (2.2.9)$$

where $p_s = ks$, and k is a cohesion increasing slope, which controls the expansion of the yield surface. M is the slope of the critical state line. Moreover,

The BBM employs a non-associated flow rule for the yield curve:

$$\frac{d\varepsilon_s^p}{d\varepsilon_{vp}^p} = \frac{2q\alpha_p}{M^2(2p + p_s - p_0)} \quad (2.2.10)$$

where α_p is a model constant, ε_s^p is the plastic deviatoric strain and ε_{vp}^p represents the plastic volumetric strain. Moreover, the elastic strains induced by changes in q are given below:

$$d\varepsilon_s^e = \frac{2}{3}(d\varepsilon_1^e - d\varepsilon_3^e) = \frac{1}{3G}dq \quad (2.2.11)$$

2.3 Macro-Micro Relations

2.3.1 Stress Tensor

Studying the micro-structural definition of the stress tensor has been the priority of different types of multi-scale investigation ([Li and Yu, 2011](#)). Under static conditions, the stresses applied to the material boundaries are transmitted through the internal structure and balanced by the interparticle interactions ([Love,](#)

1927; Bagi, 1996). Assuming a granular material as an assembly of granulates with only point contacts, the macro stress tensor can firstly be expressed as:

$$\sigma_{ij} = \frac{1}{V} \sum_{c \in V} v_i^c f_j^c \quad (2.3.1)$$

where σ_{ij} is the average stress tensor over the total volume V , f_i^c stands for the contact forces, v_i^c is the contact vector and is usually defined as pointing towards the particle center from the contact point. More specific investigations have been carried out in recent years including the consideration of dynamic effects (De Saxce *et al.*, 2004). Based on previous studies, Li *et al.* (2009) firstly presented a generalized expression of the stress tensor under a uniform stress state. The expression is derived based on Newton's second law of motion and thus can be applied in DEM simulations:

$$\overline{\sigma}_{ij} = \frac{1}{V} \left(\sum_{P \in V} \sum_{c \in P} v_i^{Pc} f_j^{Pc} + \sum_{P \in V} R_{ij}^P \right) \quad (2.3.2)$$

where v_i^{Pc} stands for the vector from the contact point c to the particle centre P , f_i^{Pc} is the force acting on the contact point c , $\sum_{P \in V} R_{ij}^P$ is a rotation term. This equation is defined as the micro-structural expression of the stress tensor. As the derivation is based on Newton's second law of motion, it is valid for both static and dynamic investigations in 3-dimensions.

2.3.2 Strain Tensor

Compared to the stress tensor, more debate exists on the macro–micro relation for the strain tensor. Research has shown that the expression of the strain tensor in micro-scale depends on the geometrical system that determines the internal structure (Li *et al.*, 2009). Bagi (1996) presented the micro-structural expression

of the strain tensor on a tessellation consisting of only simplexes. However, specific requirements of the geometry system are demanded for these expressions. Li *et al.* (2009) introduced a more generalized expression, which is valid for both polygonal (2D) and polyhedral (3D) subdivision of the granular materials. In a uniform strain field, the mean displacement gradient tensor over the total volume V could be expressed as:

$$\overline{e}_{ij} = \frac{1}{V} \oint_V e_{ij} dV = \frac{1}{V} \oint_V u_j n_i(x) dS \quad (2.3.3)$$

where V is the volume of the domain, $n(x)$ is the inwards normal direction of the boundary surface at point x , dS' is referred as the area increment of the contact surface. Using direction n as its normal direction, the area increment can be expressed by applying the divergence theorem (Li *et al.*, 2009):

$$dS' = \frac{1}{2} \oint_L ds n \cdot (x \cdot dx) \quad (2.3.4)$$

Based on the compatibility conditions, the strain tensor in micro-scale is described by:

$$\overline{e}_{ij} = \frac{1}{V} \sum_{M \in V} \sum_{S^M} \sum_{L \Delta S} \chi_i \Delta u_j \quad (2.3.5)$$

Equation 2.3.5 is the expression of the displacement gradient tensor in micro-scale. It has been proved as valid in 3D space for any polyhedral granulates. The micro-structural expression of the strain tensor therefore can be obtained as:

$$\overline{\varepsilon}_{ij} = \frac{1}{2} (\overline{e}_{ij} + \overline{e}_{ji}) \quad (2.3.6)$$

2.3.3 Capillary Stress Tensor

As a low saturation degree (pendular regime) is considered in this project, it can be assumed that capillary bridges connect only two particles. In this case, a

water-induced attractive force will be developed. Scholtès *et al.* (2009) suggested describing this attractive force by a resulting capillary force which relates to the particle size and capillary bridge volume. By using the static homogenization relation firstly developed by Love (1927), the mean stress tensor can be expressed as a function of external force:

$$\sigma_{ij} = \frac{1}{V} \sum_{p \in \partial V}^N F_i^{ext,p} x_j^p \quad (2.3.7)$$

where σ_{ij} stands for the mean stress tensor within a granular assembly, the volume of the assembly is defined as V , $F_i^{ext,p}$ is referred as the external force applied to the particles p , $p \in \partial V$ indicates that $F_i^{ext,p}$ belongs to the boundary of the granular assembly, x_j^p is the coordinate of particle p . Considering the mechanical balance of each particle within the assembly, Equation 2.3.7 can be expressed as (Scholtès *et al.*, 2009):

$$\sigma_{ij} = \frac{1}{V} \sum_{p=1}^N \sum_{q=1}^N F_i^{q,p} l_j^{q,p} \quad (2.3.8)$$

where N is the number of the particles within the assembly, $F_i^{q,p}$ is the interparticle force acting on particle p from particle q and $l_j^{q,p}$ is the branch vector between particle p and q ($l_j^{q,p} = x_j^p - x_j^q$).

For unsaturated granular soils under the pendular regime, two types of force may develop between two particles. A contact force $F_{cont}^{q,p}$ exists if two particles are in contact and a capillary force $F_{cap}^{q,p}$ appears when two adjacent particles are bonded by a capillary bridge. Depending on the local geometry, capillary bridge

could develop between two granules in contact. Therefore, for any particle couple q, p :

$$F^{q,p} = F_{cont}^{q,p} + F_{cap}^{q,p} \quad (2.3.9)$$

Combining Equation 2.3.8 and Equation 2.3.9:

$$\sigma_{ij} = \frac{1}{V} \sum_{p=1}^N \sum_{q=1}^N F_{cont,i}^{q,p} l_j^{q,p} + \frac{1}{V} \sum_{p=1}^N \sum_{q=1}^N F_{cap,i}^{q,p} l_j^{q,p} \quad (2.3.10)$$

It can be observed from the equation above that the mean stress tensor can be split into two parts:

$$\sigma_{ij} = \sigma_{ij}^{cont} + \sigma_{ij}^{cap} \quad (2.3.11)$$

where σ_{ij}^{cap} is defined as the capillary stress tensor and σ_{ij}^{cont} plays the role of effective stress. Scholtès *et al.* (2009) also demonstrated that a fabric tensor, which is useful to characterize the contact anisotropy, exists in both σ_{ij}^{cont} and σ_{ij}^{cap} . Thus σ_{ij}^{cap} can be expressed involving the fabric tensor ($\frac{1}{V} \sum_{p=1}^N n_i^{p,q} n_j^{p,q}$):

$$\sigma_{ij}^{cap} = \frac{1}{V} \sum_{p=1}^N \sum_{q=1}^N F_{cap,i}^{q,p} l_j^{q,p} n_i^{p,q} n_j^{p,q} \quad (2.3.12)$$

2.4 Discrete Element Method

2.4.1 Basic Theory

Discrete element modelling (DEM), a numerical modelling technique based on a computer simulation method, can usually be applied in soil and other granular materials. Due to the particulate properties of soil materials, advanced constitutive models are required to simulate material behaviour with more complexity. Since the original publication by Cundall and Strack (1979) in a

journal of soil mechanics, applications and research based on DEM in this area have grown rapidly. Compared to the typical approach that uses a continuum mechanics framework, DEM considers explicitly the individual particles and their interactions in a granular material. It gives a better view in geomechanics from microscopic particle interactions to macroscopic soil behaviour.

A soil can be recognized as a structure with large amounts of connecting nodes, which is considered as statically indeterminate in engineering problems as forces cannot be calculated by considering the static equilibrium of the system alone. To precisely understand the soil mechanics, more sophisticated computer models, such as DEM, with consideration of the particulate scale is required to determine the forces and displacements within the assembly. Even if applying basic numerical models with ideal particle geometries, many salient soil mechanical responses can still be characterized using DEM ([O'Sullivan, 2011](#)).

DEM is a precise time-stepping algorithm based on Newton's 2nd Law of motion. It starts with basic constitutive laws between interacting particles, due to the loading changes at the boundaries, and can then simulate the response of a particle assembly in macro scale after step-by-step computations. Deduced from particle positions by the interaction law, the particle interaction forces and their resulting forces can be determined in every time step. Newton's second law is then integrated and applied through a second-order finite difference scheme to generate the newly updated particle positions. The same process will repeat several times using the particles with their latest positions, interaction forces, velocities, geometries and orientations. Figure 2.4.1.1 shows the calculation

cycle of DEM (Itasca, 2003). During the simulations in DEM, the time step is assumed to be very small such that one particle can only have interaction with its nearest neighbour particles. Moreover, the acceleration and velocity of each particle are also assumed as constant during every time step. Eventually, the sample deformation as well as the internal/external forces can be derived from the positions and resulting forces of particles and their surrounding walls.

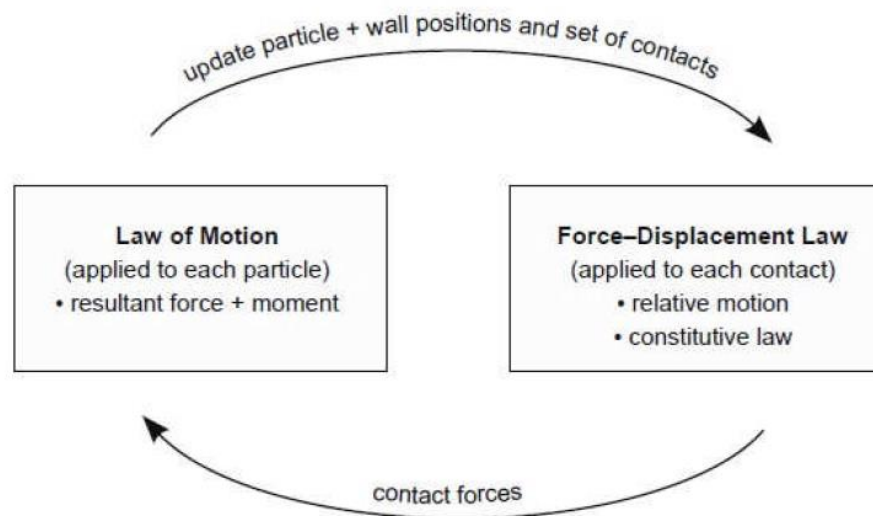


Figure 2.4.1.1 Calculation cycle of DEM (Itasca, 2003).

Two major advantages of DEM can be concluded in its application in geomechanics. Primarily, external loads and deformations can be applied in the simulation to analyse and monitor the particle-scale mechanisms underlying the macro-scale response. The evolution of particle locations, contact orientations, and contact forces can all be determined in DEM. Secondly, DEM also makes the analysis of mechanisms with large displacement possible in geomechanics. It allows us to further understand the critical failure mechanisms as the failures in geomechanics usually involve large deformation or displacement.

2.4.2 Contact Laws in DEM

To determine the contact forces includes two stages, the contact detection stage and contact resolution stage. Both are involved in DEM simulation in order to compute the contact forces. Primarily, the particles which are contacting or likely to come into contact are identified at the stage of contact detection. Values of contact forces are then calculated in an individual series of calculations. Contact forces are usually determined by cooperating virtual springs at contact points.

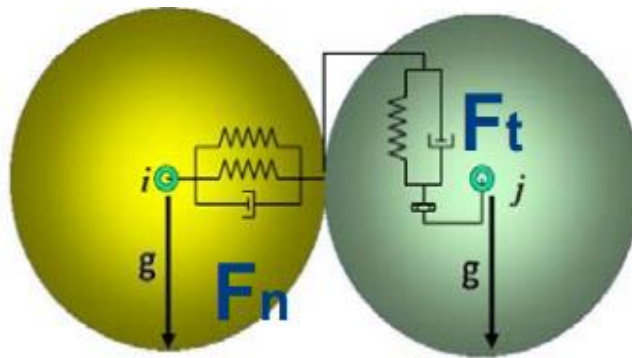


Figure 2.4.2.1 A simple soft-sphere contact model: Linear spring-dashpot (O'Sullivan, 2011).

The particles considered in DEM simulations are completely rigid, however they deform in compression in practice (O'Sullivan, 2011). Thus, by considering a small amount of overlap at contact points, the particle deformation can be simulated. Derived from the overlap depth and relative tangential motion of particles, calculations of the kinematics as well as contact geometry are carried out in the contact resolution stage. A contact constitutive model can then be specified to define the force-deformation relationship for the contact spring. The normal and tangential forces are calculated separately at contact points with two orthogonal rheological models which use combined systems of various dashpots,

springs and sliders (O’Sullivan, 2011). Figure 2.4.2.1 illustrates a simple soft-sphere contact model.

The Lagrangian method is applied to the particle phase for the integration of force balance:

$$m_p \ddot{\vec{x}}_p = \vec{F}_n + \vec{F}_t + m\vec{g} \quad (2.4.1)$$

where, F_n and F_t stand for the normal force and tangential force respectively.

The normal force tends to repulse the particles since a small overlap between particles is allowed in the simulation:

$$\vec{F}_n = -k_n \vec{\delta}_o + c_n \overline{\Delta v}_n \quad (2.4.2)$$

where, k_n is the particle normal stiffness, δ_o is the spatial overlap, c_n is the normal damping coefficient and Δv_n is the normal velocity at the contact point.

Moreover, the tangential force can be expressed as:

$$\vec{F}_t = \min \left\{ k_t \left| \int_{t_{c,0}}^t \Delta v_t(\tau) d\tau \right| \vec{t} + c_t \overline{\Delta v}_t, |\mu \vec{F}_n| \right\} \quad (2.4.3)$$

where, $t_{c,0}$ stands for the time when contact between particles starts, k_t is the particle tangential stiffness, c_t is the tangential damping coefficient and μ is the friction coefficient.

2.4.3 Implementation of Capillary Effect

As described in the previous sections, in an unsaturated soil capillary forces will be generated and applied onto the individual particles due to the surface tension developed at the air-water interfaces. It makes the unsaturated soil responses more complicated compared to those of saturated soils or dry soils. These micro

scale forces have been widely investigated as highly influential on the overall soil response (O’Sullivan, 2011).

In DEM simulations, the capillary effects in a granular assembly can be modelled using specific contact constitutive models. DEM simulation of unsaturated soil behaviour is commonly limited to the pendular regime where there is a lower degree of saturation (approximately < 20%). Capillary bridges are developed between particles in this case. Contact constitutive models are applied to determine the tensile forces resulting from the capillary bridges. A number of researchers have proposed differing contact models to represent the interparticle tensile and cohesive forces arising from the capillary effects in unsaturated soils. Soulié *et al.* (2006b) proposed a model describing the capillary bridge force as a function of contact angle, surface tension on contractile skin, capillary bridge volume and particle distance. The basic assumption in this model is that capillary force only exists within the liquid rupture distance. The rupture distance can be expressed as:

$$D_{rupture} = (1 + \frac{\theta}{2})V_{cap}^{\frac{1}{3}} \quad (2.4.4)$$

where V_{cap} is the volume of the capillary bridge, and θ refers to the water content.

2.5 LIGGGHTS

2.5.1 Introduction

LIGGGHTS stands for LAMMPS Improved for General Granular and Granular Heat Transfer Simulations. It is an open source software for modelling granular materials using the discrete element method. Different from general commercial

DEM software, this open source software allows researchers to more easily access source codes and thus improve them for specific aims. Due to the influence of capillary effects and other significant factors in unsaturated soil mechanics, it is necessary to carry out simulations on an open source software where modified contact models can be applied.

LAMMPS is a widely known outstanding open source Molecular Dynamics code published by Sandia National Laboratories (TMS, 2011). It is designed for massive parallel computations on distributed memory computers. Based on LAMMPS, LIGGGHTS is designed with enhancements to better cope with the macroscopic behaviour of the particles used in simulations. New features of LIGGGHTS relevant to unsaturated soils include non-spherical particles, importing of CAD meshes, macroscopic cohesion, stress analysis and new contact models, for example, Hertz-Mindlin and Linear Hooke.

2.5.2 Input Scripts

Since LIGGGHTS is an improved granular package based on LAMMPS, it recognizes the same input scripts as LAMMPS. In DEM software, input scripts are usually used for simulation setup and simulation output. Generally, they consist of four parts: initialization, atom definition, settings and running a simulation. The first two parts define the particle topology and the last two steps can be repeated multiple times during a simulation.

At the stage of particle initialization, different basic parameters of particles such as units, dimension, boundary and style of particle can be firstly set up. Particles

then need to be further defined by creating particles on a lattice, or reading data from a data file. In LIGGGHTS, moreover, a variety of settings can be applied for granular materials, for example, force field coefficients, material properties, simulation parameters and output options. Force field coefficients are related to the particle contact models in some circumstances, and they can be computed based on the material properties. After complete editing of the input scripts the LIGGGHTS simulations would be started by specifying the run command for the total number of steps.

2.5.3 Contact Models in LIGGGHTS

Due to the significance of capillary effects in unsaturated soil behaviour, the choice of contact model can be regarded as the priority in subsequent simulations. Compared to LAMMPS, the contact models in LIGGGHTS offer advantages as they allow the stiffness (k_n, k_t) and damping coefficients (γ_n, γ_t) to be derived from the material properties. In this case, multiple fixes of type global/property are mandatory to define the material properties.

Hertz-Mindlin and the Linear-Hooke are the most commonly used contact models in LIGGGHTS, and now both are enhanced with macroscopic cohesion. After determining the parameters, normal and tangential forces between particles can be calculated using equations 2.4.2 and 2.4.3.

2.5.3.1 Hertz-Mindlin contact model

In the Hertz-Mindlin contact model, the normal particle stiffness (k_n) and damping coefficients (γ_n) are calculated by:

$$k_n = \frac{4}{3} E^* \sqrt{R^* \delta_n} \quad (2.5.1)$$

$$c_n = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_n m^*} \quad (2.5.2)$$

where,

$$S_n = 2E^* \sqrt{R^* \delta_n} \quad (2.5.3)$$

$$\beta = \frac{\ln(e_r)}{\sqrt{\ln^2(e_r) + \pi^2}} \quad (2.5.4)$$

$$\frac{1}{m^*} = \frac{1}{m_1} + \frac{1}{m_2} \quad (2.5.5)$$

$$\frac{1}{R^*} = \frac{1}{R_1} + \frac{1}{R_2} \quad (2.5.6)$$

$$\frac{1}{E^*} = \frac{(1 - v_1^2)}{E_1} + \frac{(1 - v_2^2)}{E_2} \quad (2.5.7)$$

where, m and R stand for particle mass and radius, respectively, v is the particle Poisson ratio and E is the particle Young's Modulus, k_n is the particle normal stiffness, δ_n is the particle overlap.

In equation 2.5.2, c_n is the particle normal damping coefficient. e_r is the coefficient of restitution, referring to the ratio of speeds after and before an impact. The superscripts stand for the number of particles. Moreover, the tangential particle stiffness (k_t) and damping coefficient (c_t) can be calculated by:

$$k_t = 8G^* \sqrt{R^* \delta_n} \quad (2.5.8)$$

$$c_t = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_t m^*} \quad (2.5.9)$$

where,

$$S_t = 8G^* \sqrt{R^* \delta_n} \quad (2.5.10)$$

$$\frac{1}{G^*} = \frac{2(2 + \nu_1)(1 + \nu_1)}{E_1} + \frac{2(2 + \nu_2)(1 + \nu_2)}{E_2} \quad (2.5.11)$$

2.5.3.2 Linear-Hooke contact model

In the Linear-Hooke contact model, the particle stiffness and damping coefficients have the same values in normal and tangential directions, and are calculated as:

$$k_n = k_t = \frac{16}{15} \sqrt{R^* E^*} \left(\frac{15 m^* v^2}{16 \sqrt{R^* E^*}} \right)^{\frac{1}{5}} \quad (2.5.12)$$

$$c_n = c_t = \sqrt{\frac{4 m^* k_n}{1 + \left(\frac{\pi}{\ln(e_r)} \right)^2}} \quad (2.5.13)$$

To better understand the capillary effect in unsaturated soil mechanics, both the Linear-Hooke model and the Hertz-Mindlin model will be applied in the simulations. Either one may be used in the final study after comparing their accuracy.

2.6 X-ray Computed Tomography

2.6.1 Basic Features

The mechanical behaviour of unsaturated granular soil is significantly dependent upon the soil microstructure which includes shape, arrangement and distribution of particles, liquid and void space within a soil material. With the scanning technique, a digital image can be created by measuring the X-ray linear attenuation coefficient of an object, which is dependent on the density of a material (Nielsen, 2004). Materials with different densities thus will present a

different appearance under X-ray CT scanning. Normally a high density-material will attenuate more X-rays than a material with lower density. During the past decade, many studies have been conducted to measure soil properties at microscale, including void ratio, physical density, particle size distribution, etc. (Tollner *et al.*, 1998; Nielsen, 2004). These research studies have proven some capabilities and advantages of X-ray CT in measuring the soil microstructure. Its application in geotechnical engineering is still in an early stage, however the rapidly developing technology has driven increasing number of researchers to study and investigate in this area.

Compared to traditional methods, the major advantages of X-ray CT include minimal sample disturbance and time savings. A study by Tollner *et al.* (1998) showed that X-ray scanning can provide particle size data consistent with the traditional methods, but without adopting the sample coupon preparation. Due to the minimal disturbance during scanning, X-ray CT also allows a granular sample to be scanned multiple times. This superiority makes it possible for the investigation of particle and pore interactions at any time or location within a soil sample. In this study, a cylindrical container with glass beads will be scanned and studied using the X-ray CT technique. This method will be used to determine the geometry and the spatial distribution of capillary bridges within a granular assembly.

2.6.2 Scanning Process

In the first stage of X-ray CT scanning, the specimen will be photographed from different multiple angles while being exposed to X-ray beams. Different

amounts of X-rays will be absorbed when passing through materials with different densities. It is found that denser materials such as rock and sand can absorb more X-rays than materials with lower densities such as water (Nielsen, 2004). X-rays will finally pass through the specimen, and illuminate a detector screen within the apparatus. The image on screen will then be recoded with a digital camera to replicate the penetration pattern of the specimen. Multiple viewing angles are required to obtain complete information for a complex material which contains various internal features. In the data collection phase, the X-ray penetration pattern is constituted by collecting and combining many slices of individual images scanned from the specimen. Russ (2002) noted that the specimen is required to be photographed while rotating at least half of a full rotation relative to the location of the sensitive screen and the X-ray trajectory. It is sufficient to collect views within 180° as all the possible interior characteristics and combinations can be completely presented in a half rotation. Nielsen (2004) also reported that using a closer detecting view around the rotation can lead to a finer image resolution. Reconstruction after X-ray CT scanning can provide a representation of the internal features of the specimen. The X-ray images from different views through the cross-section are used to determine the precise locations of the interior structures.

2.6.3 Digital Image Processing

A digital image is a picture converted to numerical form for it to be processed and stored in a computer. As illustrated in Figure 2.6.3.1, the fundamental constituent elements in digital images are commonly defined as a pixel (1x1 square) in 2D and a voxel ($1 \times 1 \times 1$ cube) in 3D (Manahiloh and Meehan,

2017). Images of higher quality can be produced when a larger number of pixels is applied. The intensity of an image at a specific point can be represented by the value of each pixel or voxel.

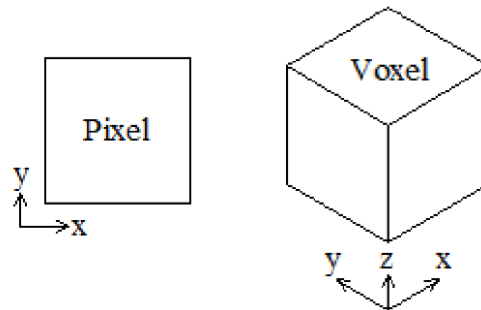


Figure 2.6.3.1 Illustration of a pixel in 2D and a voxel in 3D (Manahiloh and Meehan, 2017).

Digital images can commonly be classified into four categories, which are binary images, grayscale image, color images and multipicture images. Binary images are also known as black-white images. Only two values, *i.e.* either '0' or '1' are taken account in a binary image. Geometric information of an object, such as the location of its centroid, the orientation and the profile of the object can be extracted from a binary image.

Figure 2.6.3.2a shows an example of a binary image (Jayaraman *et al.*, 2009). A grayscale image contains only brightness information, in which each pixel represents only the quantity of light. A grayscale image can be converted to binary by a thresholding operation. In contrast to the binary image, brightness graduation can be alternated in a grayscale image. Each pixel in the grayscale image is represented by a byte, the value of which is used to represent the light intensity at the corresponding point of the image. As illustrated in Figure

2.6.3.2b, an 8-bit grayscale image has a brightness variation from 0 to 255 where black is represented by 0 and white is defined as 255 (Jayaraman *et al.*, 2009).

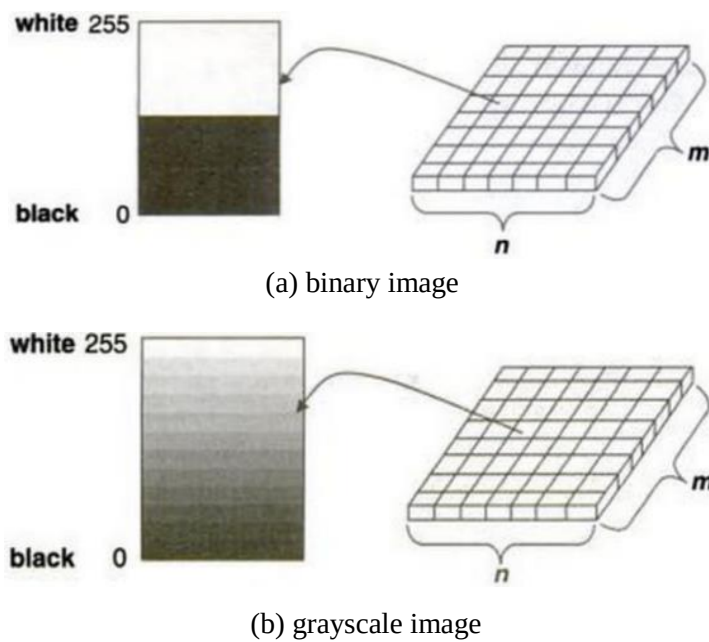


Figure 2.6.3.2 Explanation of binary image and grayscale image (Jayaraman *et al.*, 2009).

Furthermore, a colour image has three values per pixel, and commonly consists of three independent colour planes. The pixel values in each plane represent the intensity of the corresponding colour at a specific point in the image. RGB, as the most widely used colour image system, uses red, green and blue to define the intensity of various colours.

Digital image processing commonly consisted of a series of algorithms for solving different problems, such as noise reduction, contrast improvement, object recognition and segmentation, and many other qualitative analyses (Razavi, 2007). Applications of digital image processing have been conducted in various subjects, including engineering, medicine and natural science studies.

In geotechnics, digital image processing has been adopted to investigate various subjects including the hydraulic properties, pore network features, and the mechanical behaviour of soils ([Otani and Obara, 2004](#); [Taina, 2008](#); [Périard et al., 2016](#)). It has been proved to be applicable in determining the numbers, sizes, and orientations of soil particles, quantifying the porosity and anisotropy, analysing the distribution of pores and particles, *etc.* ([Jayaraman et al., 2009](#)).

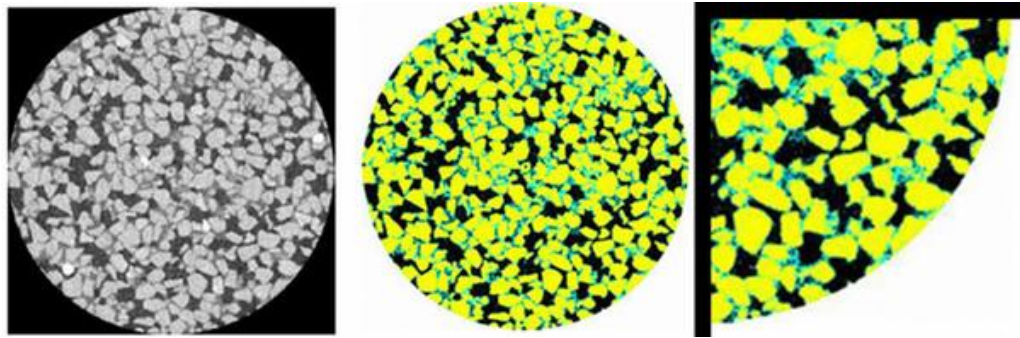


Figure 2.6.3.3 Microstructure of unsaturated soil under XRCT, (blue: water phase, yellow: soil particles, black: pore space) ([Yosuke, 2013](#)).

In many theoretical models, the pore water is assumed to distribute homogeneously and only to exist at particle contact points ([Smith et al., 1929](#)). However, current image processing carried out using X-ray CT shows the heterogeneous distribution of capillary bridges in unsaturated glass granulates ([Endo et al., 1992](#); [Endo et al., 1993](#)). It is also proved that cohesion also exists between nearby non-contact particles. Figure 2.6.3.3 presents cross sections of the microstructure of an unsaturated soil material acquired by X-ray CT after image processing, where the water phase is highlighted as blue, the yellow and black phases refer to soil particles and pore space respectively. Microscopic observations can provide qualitative information on the pore water in unsaturated granular materials. It also indicates that differences between theoretical values and experimental results might be caused by the

heterogeneous distribution of pore water and capillary bridges. Different algorithms of digital image processing are applied in this study to mainly investigate the local geometries and spatial distribution of capillary bridges under low water contents. Results will also be compared with the microscopic information generated in DEM.

2.6.4 Avizo Fire v8.1 Software

Avizo Fire v8.1 software is a modular and object-oriented software system developed by Thermo ScientificTM, and it is based on the latest release of Open Inventor by Visualization Sciences Group. Avizo mainly focuses on the modelling, visualization and analyses of digital images in 3D. It can be applied for data analysis in a vast range of subjects, including archaeology, astrophysics, physics, chemistry, scientific visualization, *etc.* Numerous research studies in image processing have been carried out with Avizo. Its application in geotechnics and material sciences has increased during the past decade ([Tracy et al., 2010](#); [Keller et al., 2011](#); [Yang et al., 2013](#); [Zacher et al., 2014](#); [Rogers et al., 2016](#)).

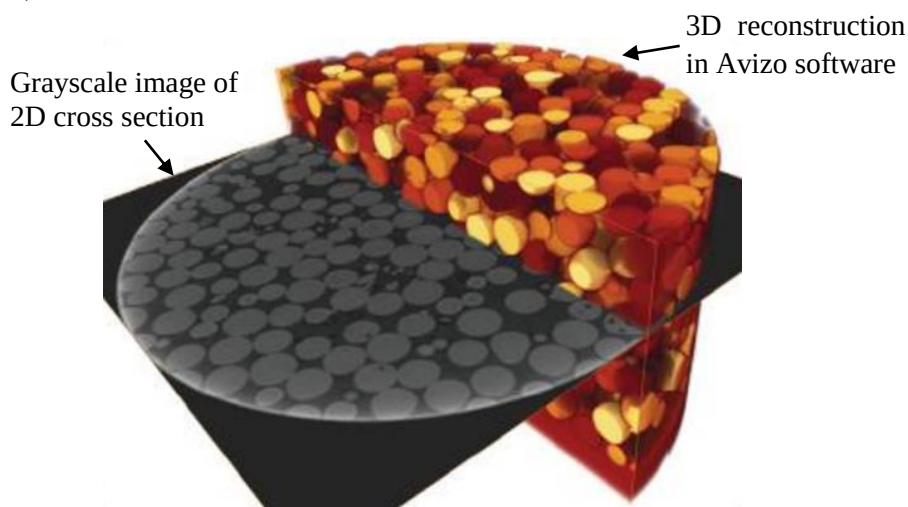


Figure 2.6.4.1 Grayscale images of glass powder processed and rendered in Avizo Fire software ([Visualization Sciences Group, 2013](#)).

Images from computed tomography and microscopy can be accessed and analysed with Avizo. Thus, it can be used for better characterization of unsaturated material and its internal structure. Pore network characterization and particle analysis can be operated to quantify the pores or particles in the material, as well as their shapes and volume distributions. Computation of material physical properties such as porosity and permeability can also be implemented. Figure 2.6.4.1 shows a 3D image of glass powder segmented and rendered in Avizo, along with a random slice of the grayscale image ([Visualization Sciences Group, 2013](#)).

The basic components of the Avizo system consist of modules and data objects. Modules are used for visualization and numerical computations of the data objects. Direct OpenGL rendering is applied in several modules to achieve special rendering effects or performance enhancement. The components are represented by small icons in the Project View in Avizo. These icons are linked with lines indicating the modules applied with the corresponding data objects. Parameters of data objects and modules can be customized in the interaction area in Avizo. Some interactive editors with special purposes are also incorporated for the modification of specific data objects, such as colormaps. More than 270 types of module and data objects are available in Avizo, allowing visualization, analysis and modelling of 3D data of various types. The advanced workflow in Avizo is optimal for the integration and analysis of data from multiple sources.

2.7 Summary

From this chapter, it can be found that for an unsaturated soil system in equilibrium, external pressure can be balanced by the components of pressure and stress due to the phases and their interactions. These components consist of the interaction between soil particles, the meniscus formed at the water-air interface, water and air pressure, water vapour in air, dissolved air in water, and the pressure on soil particles arising from the surrounding liquid. For the pendular regime, previous research has proven that applying capillary theory can efficiently relate the capillary bridge force with the local geometry of the particles and the capillary pressure. It is agreed that SWRC relates the water content of a soil to its matric suction and is a significant hydraulic property related to the size and connectivity of the soil microstructure. Different models with fractal pore-water distributions have been proposed recently to predict the SWRC. In this project, further investigations will be carried out mainly focusing on quantity and spatial distribution of capillary bridges, which are dependent on the polydispersity and the anisotropy of the particle arrangement.

In DEM, the mechanical behaviour of unsaturated granular materials can be determined by including local interactions in numerical simulations. With the newly implemented contact models in LIGGGHTS, the capillary cohesion and matric suction can be simulated to study the macro-micro relations. By adopting different types of particles with the toroidal approximation for the capillary bridge geometries, a modification of inter-particle force distribution can be proposed to investigate the influence of water distribution in unsaturated granular material. Suction-controlled triaxial compression tests can be carried

out to relate matric suction with capillary bridge distribution. Experiments with X-ray CT can be conducted to analyse the spatial distribution and local geometries of capillary bridges in unsaturated specimens with low water contents. Validation of the capillary bridge model in DEM thus can be carried out according to the practical observations.

CHAPTER 3: Computational Techniques and Experimental Methodology

3.1 Introduction

By the discrete element method (DEM), the behaviour of wet granular materials can be predicted by including local interactions in numerical simulations. DEM was initially developed to simulate the behavior of dry granular materials according to the direct relations between external loads and the interparticle forces ([Cundall and Strack, 1979](#)). As there are good agreements between experimental observations and DEM simulations, it has recently become a popular tool and evolved into a mature technique for wet granular materials. In this study, dry triaxial test simulation was firstly carried out to study the microscopic parameters including rolling coefficient and friction angle. The numerical model has then been calibrated to match the experimental results from previous publications.

Using the toroidal approximation method developed by Wang ([2014](#)), the capillary effect was implemented between two spherical particles. Suction controlled triaxial test simulations were later conducted using numerical assemblies with uniform water distribution. The capillary strengthening effect of unsaturated granular materials in the pendular state could be confirmed. The mechanical behaviour of unsaturated granular soil is significantly dependent upon the soil microstructure which includes geometric information, arrangement and distribution of particles, liquid and void space within a soil material.

Numerous studies have been carried out focusing on some of these factors, such as particle size distribution and unique particle shape. However the liquid phase was commonly assumed to be uniformly distributed in previous studies. Since only a low level of water content is involved in the pendular state of unsaturated material, a random distribution of water thus is more likely to be encountered in practical problems. To study and understand the influence of water distribution in an unsaturated granular material, different distribution models for capillary effects are presented in this study. By modelling monodisperse packings incorporating with defined rules of water distribution and the elementary laws under external loadings, macroscopic behaviour and the stress-strain relationship of unsaturated soil can be more accurately simulated with increasing water content.

To further study and better interpret the mechanical behaviour of unsaturated soil, both numerical modelling and experimental observations are presented in this project. X-ray CT scanning allows researchers to obtain 3D information of materials at mesoscale, and achieve characterization of unsaturated soil microstructure ([Bruchon, 2013](#); [Scheel et al., 2008](#)). Monotonic glass beads of 0.5mm diameter have been scanned with low saturation degrees ($S_r = 6\%, 9\%$ and 12%). Avizo was later applied for image processing. To investigate the effects of pore size, packing density and geometry of capillary bridges, each phase of the unsaturated assembly was segmented using the thresholding technique. Contacting particles could also be disconnected using a watershed algorithm. Particle size distribution of the unsaturated specimens was analysed by labelling each disconnected object, and calculating the volume of

each label. Distribution of capillary bridges was estimated by segmenting the image into various cube units, and determining the saturation degree within each unit. Using the volume rendering in Avizo, geometric information of capillary bridges was later evaluated and compared to the numerical model.

3.2 Numerical Simulation Method

3.2.1 LIGGGHTS

LIGGGHTS stands for ‘LAMMPS improved for general granular and granular heat transfer simulations’. As an open source software, it was first developed by Kloss *et al.* (2012). LIGGGHTS is a special package of the molecular dynamic software LAMMPS, focusing on modelling granular material problems. It is selected in this study due to its particular features including cohesion models, rolling stiffness models and normal and tangential contact models.

3.2.2 Dimensionless Interpretation in DEM

By following the dimensionless study proposed by Wang (2014), the dimensionless contact force (F^d) can be expressed as:

$$F^d = \frac{F}{R^2 E} = f\left(\frac{\delta_n}{R}, e, \mu\right) \quad (3.2.1)$$

where $\frac{\delta_n}{R}$ refers to the particle strain, e is the void ratio and μ is defined as the friction coefficient. The dimensionless stress tensor is defined by:

$$\sigma_{ij}^d = \frac{\sigma}{E^*} = f\left(\frac{\bar{R}^3}{V}, C_u, C_c, \frac{\delta^c}{\bar{R}}, u^c, \frac{e_i^c}{\bar{R}}, n_j^c, t_j^c\right) \quad (3.2.2)$$

where $\bar{R}$ is the mean particle radius and V stands for the volume of the assembly, C_u and C_c are adopted as the coefficients defining the PSD, $\frac{\delta^c}{\bar{R}}$ is the mean

interparticle strain, u^c is the friction mechanism and $\frac{v_i^c}{R}, n_j^c, t_j^c$ refer to the dimensionless form of internal fabric. E^* is the effective Young's modulus.

3.2.2.1 Hooke contact

In the linear Hooke contact model, the normal contact force is defined as:

$$F_n = k_n \delta_n \quad (3.2.3)$$

According to Equation 3.2.1, the dimensionless contact force in the linear Hooke contact model can be determined by:

$$F^d = \frac{F}{R^2 E^*} = \frac{k_n \delta_n \sqrt{1 + \mu^{c2}}}{R E^*} = \frac{k_n}{R E^*} \frac{\delta_n}{R} \sqrt{1 + \mu^{c2}} \quad (3.2.4)$$

where $\frac{k_n}{R E^*}$ is a dimensionless term and the dimensionless contact force in Equation 3.2.4 is only dependent on $\frac{\delta_n}{R}$ and μ^c . To represent the similar material property with different particle sizes it can be found that $k_n \propto R E^*$. By following the form of the dimensionless stress tensor and substituting the average contact stiffness of the granular assembly, the dimensionless stress tensor for the Hooke model can be expressed as:

$$\sigma_{ij}^d = \frac{\sigma_{ij}}{E^*} = \frac{\sigma_{ij} \bar{R}}{k_n} = \frac{\bar{R}^3}{V} \sum_{c \in V} \frac{\delta^c}{\bar{R}} \frac{v_i^c}{\bar{R}} (n_j^c + \mu^c t_j^c) \quad (3.2.5)$$

3.2.2.2 Hertz contact

In the Hertz contact mechanism (Johnson, 1987), the contact force is defined as:

$$F_n = \frac{4}{3} R^2 E \left(\frac{\delta_n}{R} \right)^{3/2} \quad (3.2.6)$$

According to Equation 3.2.1, it can be derived that:

$$k_n = \frac{3}{4} E^* \sqrt{R \delta_n} \quad (3.2.7)$$

where k_n is no longer a constant in the Hertz contact but related to the particle deformation. Thus, the mean contact stiffness ($\overline{k_n}$) in a particle assembly with Hertz contact model can be defined using the mean particle size ($\bar{R}$) and mean overlap distance ($\bar{\delta_n}$):

$$\overline{k_n} = \frac{3}{4} E^* \sqrt{\bar{R} \bar{\delta_n}} \quad (3.2.8)$$

By substituting into the dimensionless stress expression (Equation 3.2.2), the dimensionless stress tensor for the Hertz contact model can be expressed as:

$$\sigma_{ij}^* = \frac{\sigma_{ij}}{E^*} = \frac{\sigma_{ij} \bar{R}}{k_n} = \frac{\bar{R}^3}{V} \sum_{c \in V} \frac{\delta^c}{\bar{R}} \frac{v_i^c}{\bar{R}} (n_j^c + \mu^c t_j^c) \sqrt{\frac{\delta^c}{\bar{\delta}}} \sqrt{\frac{2R^c}{\bar{R}}} \quad (3.2.9)$$

where R^c is the equivalent contact radius at the contact point c .

It can be found that in a monodispersed particle system, the contact overlapping probability distribution ($\sqrt{\frac{\delta^c}{\bar{\delta}}}$) is the only parameter that may distinguish the dimensionless stress conditions for the two models. For a particle assembly with a wide particle size distribution, however, significant influences can be caused by the terms $\sqrt{\frac{\delta^c}{\bar{\delta}}}$ and $\sqrt{\frac{2R^c}{\bar{R}}}$. To achieve a more comprehensive simulation method including the consideration of a wide particle size distribution, it is important to investigate the effect of particle size distribution on the two contact models.

3.2.3 Rolling Resistance Models

3.2.3.1 Basic features

Since spherical particles are used in the simulations to keep a low calculation cost, the local constitutive law of conventional DEM was modified using an additional component at each contact point where rolling resistance was introduced. This is regarded as the rolling resistance model. Rolling resistance refers to a couple which can be transferred between a pair of particles via the contacts, and it is produced to resist particle rotation. It has previously been demonstrated that rolling resistance in DEM simulations of spherical particles is a viable approach ([Belheine, 2008](#); [Jiang *et al.*, 2006](#)). Real grains are normally not spherical and generally they present a rough surface texture. Reports have shown that they can be covered with a thin film of weathered products ([Iwashita and Oda, 1998](#); [Zhou *et al.*, 1999](#)). In practice grains get in contact with their neighbours through this contact surface instead of a single point. In this case, rolling resistance can play a significant role on the contact behaviour of the spherical medium.

With the rapid development of DEM in recent years, the importance of rolling resistance, particularly in simulation of spherical particles has been gradually realized and studied by researchers. Different rolling resistance models have been proposed, however there are crucial differences between them. This may be attributed to the fact that these models were proposed for the investigation of different specific problems and the rolling resistance can be generated from various sources.

The kinematics of two 2D spheres in contact was firstly implemented into DEM by Iwashita and Oda (1998) and then improved by Jiang *et al.* (2005; 2006). Further work on both 2D and 3D particles with irregular shapes has been proposed by Kuhn *et al.*, (2002), and Kuhn and Bagi (2003; 2004a; 2004b). Based on the models reported by Feng *et al.* (2002) and Iwashita and Oda (1998). Li *et al.* (2005) proposed a study on DEM modelling of the failure modes of granulates including the effect of rolling resistance. The tangential friction force in this model is also separated into a rolling component and a sliding component. In this model, two tangential force components are related to their corresponding relative movements and different stiffnesses. As a result its application requires the determination of more parameters.

3.2.3.2 Coefficient of rolling resistance

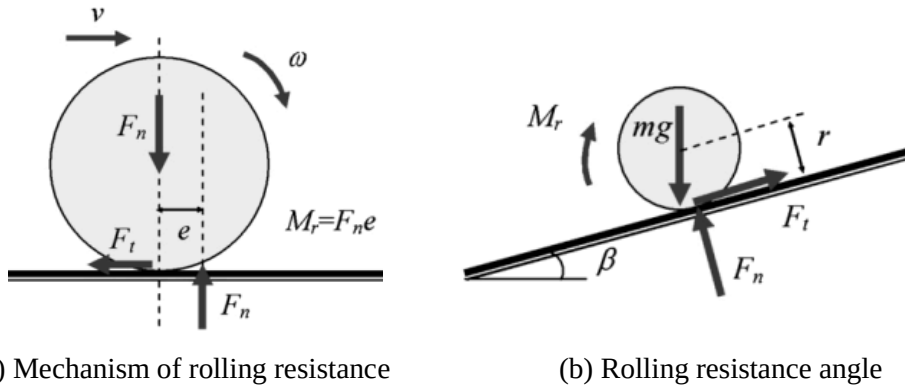
While a spherical particle is rolling, the normal contact pressure on the contact surface redistributes continuously. As a result, an eccentricity e_e is developed from the consequent normal force towards the rolling direction with regard to the stationary contact point, and it would generate a resistance moment M_r (Figure 3.2.3.1a). However, different definitions of rolling friction have been adopted in the previous DEM studies. The eccentricity e , which has a unit of length, is commonly regarded as the coefficient of rolling friction (Lakshmana *et al.*, 2003; Goriacheva, 1998). Other studies considered e as a parameter with two components including a length parameter and a dimensionless parameter which is taken as the coefficient of rolling friction (Iwashita and Oda, 2000; Li *et al.*, 2005; Feng *et al.*, 2002). In this study a definition with a clear physical

meaning is adopted. The term “coefficient of rolling resistance” μ_r is adopted, and μ_r is defined as a dimensionless parameter:

$$\mu_r = \tan(\beta) \quad (3.2.10)$$

where β is defined as the angle of rolling resistance.

By considering an object on a slope, Figure 3.2.3.1b shows the definition of β which is the maximum angle of a slope, where the rolling resistance torque counterbalances the torque developed by gravity acting on the body (Ai *et al.*, 2011).



(a) Mechanism of rolling resistance

(b) Rolling resistance angle

Figure 3.2.3.1 Illustrations of rolling resistance mechanism and rolling resistance angle. (Ai *et al.*, 2011).

3.2.3.3 Rolling stiffness

In many rolling resistance models, the rolling stiffness k_r can be a crucial parameter. Iwashita and Oda (1998) proposed that rolling stiffness can be expressed as:

$$k_r = k_n R_r^2 \quad (3.2.11)$$

where k_n is the tangential contact stiffness. In this model it is assumed that the torque caused by the sliding component and rolling component are of the same order.

3.2.3.4 Relative particle rotation and rolling radius

Previous research has also indicated the importance of the rolling radius and relative particle rotation (Ai *et al.*, 2011). These two parameters are defined by determining the kinematics of a pair of particles in contact. By considering two spherical particles A and B , with radii r_A and r_B respectively, Figure 3.2.3.2 shows their kinematics in contact during the time increment from t to $t + dt$.

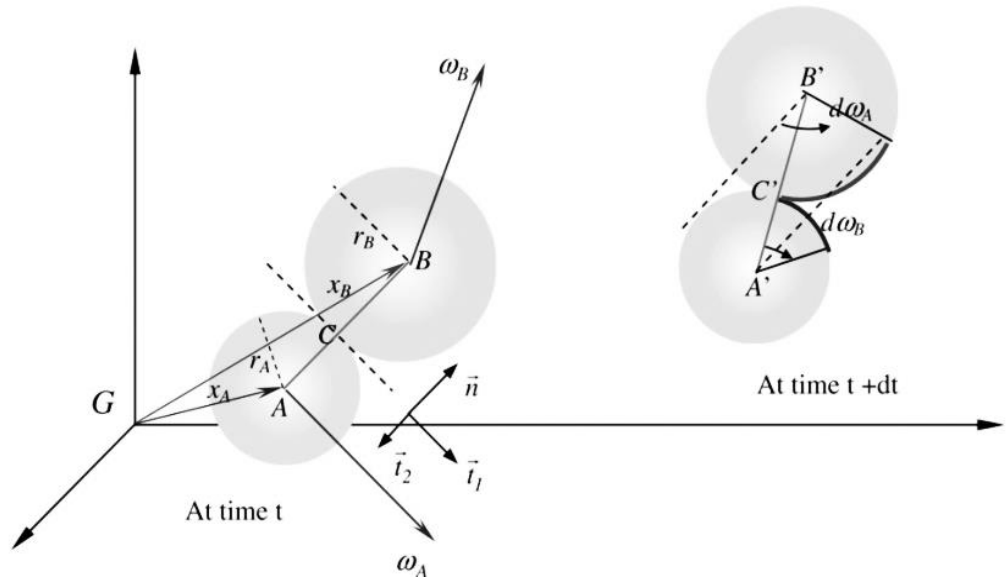


Figure 3.2.3.2 Kinematics of two spherical particles in contact at times t and $t + dt$ (Ai *et al.*, 2011).

It is assumed that they remain in contact during a time step. x_A and x_B refer to the position vectors of the particle centres in the global axes O. ω_A and ω_B denote their rotations, while $\dot{\omega}_A$ and $\dot{\omega}_B$ are the rotation velocities. $d\omega_A$ and $d\omega_B$ refer to the incremental rotations which take place during the time increment. n and n'

denote the unit vectors at time t and $t + dt$ respectively, and they are normal to the tangential plane of the contact point C and C' . The new position is defined by the vectors x_A' and x_B' .

The relative rolling between the two particles can be identified by determining the incremental rotation and the sliding component. Then the incremental displacement vector can be expressed in terms of the relative position. Only rolling occurs without any particle sliding at the contact if the components of relative sliding equal zero, while pure sliding occurs if the incremental rotation is zero. The incremental trace can be found as:

$$dS_A = r_A(d\theta_A + d\varphi) \quad (3.2.12)$$

$$dS_B = r_B(d\theta_B - d\varphi) \quad (3.2.13)$$

where $d\varphi$ is the incremental change of the angle of contact direction between two particles, $d\theta_A$ and $d\theta_B$ denote the incremental rotations of particles A and B , dS_A and dS_B are both composed of the rolling and sliding components dU_r and dU_s :

$$dU_r = (r_B dS_A - r_A dS_B) / (r_A + r_B) \quad (3.2.14)$$

$$dU_s = (dS_A + dS_B) / 2 \quad (3.2.15)$$

Combining Equation 3.2.6 and 3.2.8, the relative rotation between the two particles $d\omega_r$ can be determined as:

$$d\omega_r = d\omega_A - d\omega_B = \frac{dU_r}{R_r} \quad (3.2.16)$$

where R_r denotes the rolling radius,

$$R_r = r_A r_B / (r_A + r_B) \quad (3.2.17)$$

Equation 3.2.10 can be then expressed as:

$$d\omega_r = dU_r / R_r \quad (3.2.18)$$

3.2.3.5 Elastic-plastic spring-dash model

The torque in elastic-plastic spring-dash (EPSD) models generally consists of two components which are the mechanical spring torque and the viscous damping torque. In the models proposed by Iwashita and Oda (1998) and Jiang *et al.* (2005), the mechanical spring torque can be determined by the relative rotation between two particles. Based on their models, Ai *et al.* (2011) developed a more versatile model which considers the simulation situations involving cyclic rolling and rolling back. In the models of this category, the total rolling resistance torque M_r consist of a spring torque M_r^k and a viscous damping torque M_r^d :

$$M_r = M_r^k + M_r^d \quad (3.2.19)$$

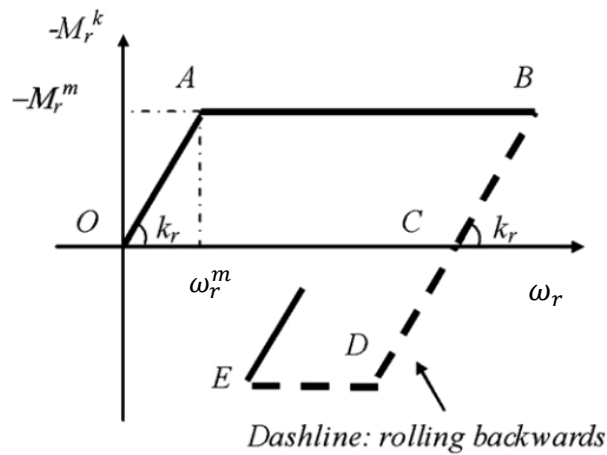


Figure 3.2.3.3 Spring torque of elastic-plastic spring-dashpot rolling resistance model (Ai *et al.*, 2011).

Figure 3.2.3.3 shows the spring torque M_r^k in this model which is similar to the loading-unloading stress-strain curve of an elastic perfectly plastic material (Ai *et al.*, 2011). The major improvement in this model is the inclusion of the rolling back curve which makes it more efficient for application in cyclic rolling problems.

By using an incremental method, this model can be easily implemented in a numerical simulation. By considering the spring torque at time t as $M_{r,t}^k$, the incremental torque dM_r^k can be found from the incremental relative rotation between two particles $d\omega_r$ and the rolling stiffness k_r .

$$dM_r^k = -k_r d\theta_r \quad (3.2.20)$$

the spring torque at time $t + dt$ can be determined as:

$$\begin{cases} M_{r,t+dt}^k = M_{r,t}^k + dM_r^k \\ |M_{r,t+dt}^k| \leq M_r^m \end{cases} \quad (3.2.21)$$

$$M_r^m = \mu_r R_r F_n \quad (3.2.22)$$

where M_r^m is defined as the limiting spring torque which is achieved at a full mobilisation rolling angle,

$$\omega_r^m = M_r^m / k_r \quad (3.2.23)$$

where ω_r^m denotes the maximum incremental relative rotation between the particles, and k_r is the rolling stiffness. The spring torque is restricted by the full mobilisation torque M_r^m which is determined by the normal force F_n and the coefficient of rolling friction μ_r . The viscous damping torque M_r^d is assumed to be dependent on the damping constant C_r and the relative rolling angular velocity $\dot{\omega}_r$ between two spheres in contact:

$$M_{r,t+dt}^d = \begin{cases} -C_r \dot{\omega}_r & \text{if } |M_{r,t+dt}^k| < M_r^m \\ -f C_r \dot{\omega}_r & \text{if } |M_{r,t+dt}^k| = M_r^m \end{cases} \quad (3.2.24)$$

The second function includes a parameter f . When $f = 1$, the viscous damping component is always presented to simulate any possible viscous dissipative interaction existing between two particles. If $f = 0$, the viscous damping torque will not be activated after the contact rolling torque is fully mobilised. Instead of dissipating a large amount of energy, the viscous damping acts as a general treatment for stabilising the sample and preventing rolling oscillation (Ai *et al.*, 2011). The rolling viscous damping coefficient C_r can be expressed as:

$$C_r = \eta_r C_r^{crit} \quad (3.2.25)$$

where η_r is the rolling viscous damping ratio and C_r^{crit} is the rolling critical viscous damping constant,

$$C_r^{crit} = 2\sqrt{I_r k_r} \quad (3.2.26)$$

where I_r denotes the equivalent moment of inertia for the relative rotational vibration mode about the contact point between the two contacting disks,

$$I_r = 1 / \left(\frac{1}{I_A + m_A R_A^2} + \frac{1}{I_B + m_B R_B^2} \right) \quad (3.2.27)$$

where I_A and I_B refer to the moment of inertia with respect to the centroid, m_A and m_B are the mass of particles A and B respectively.

An alternative EPSD model used in this study was proposed by Iwashita and Oda (1998). Different to the model proposed by Ai *et al.* (2011), the viscous damping torque M_r^d is disabled. Moreover, the rolling stiffness in this model is defined as Equation 3.2.11. Both models are used in simulations, not only for

calibration purposes but also for comparison and parameter investigation. In this study, $f = 1$ was adopted in all tests to save calculation time.

3.2.4 Cohesion Models

3.2.4.1 Basic features

The capillary bridge model used in this study was developed by Wang (2014), which used the iterative method based on the toroidal approximation of capillary bridge geometry. A constitutive law for unsaturated soil could be developed at particle scale using this method. For unsaturated granular material modelled by DEM, several hypotheses are established to describe the physical characteristics of solid particles and capillary bridges. Firstly, particles are assumed to be spheres with smooth surfaces. The menisci of the capillary bridges are considered as arcs, and are also in a predominantly concave shape. It is also assumed that identical liquid-particle contact angles (θ_1 and θ_2) with a difference less than $\frac{\pi}{1800}$, are developed for each pair of particles bonded by the capillary bridge. The self-weight of the numerical assembly under gravity was also neglected as significantly greater interparticle forces were developed from the boundaries. The self-weight of water was also eliminated due to the small volume of the capillary bridge.

Furthermore, the liquid viscosity was also ignored in this method as the granular material deformation could satisfy the quasi-static condition. Figure 3.2.4.1 illustrates the conceptual capillary bridge with a pair of spherical particles, which comply with the assumptions above. It shows that the x axis passes through the

particle centroids and the y axis crosses the middle point of the interparticle gap. The capillary bridge is thus assumed to be symmetrical to the x axis. xc_1 and xc_2 are the x co-ordinates of the intersection points of liquid surface and particles. β_1 and β_2 refer to the half-filling angles in the particles.

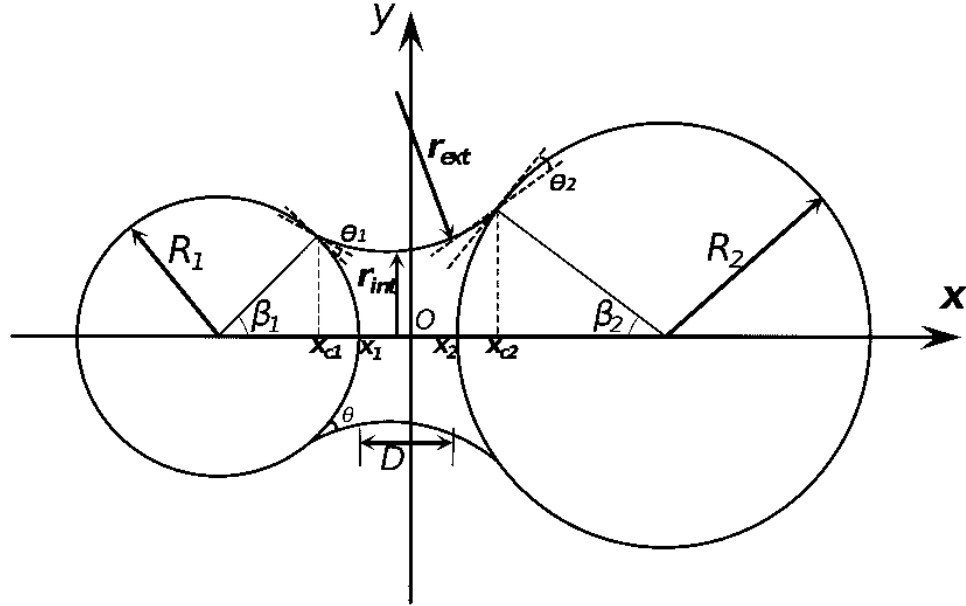


Figure 3.2.4.1 Geometric information of capillary bridge.

By the Young-Laplace equation, the matric suction is defined as the difference between water and air pressure. It is also dependent on the curvature of the capillary bridge and the surface tension (T) of the liquid:

$$S = T \left(\frac{1}{r_{ext}} - \frac{1}{r_{int}} \right) \quad (3.2.28)$$

where S is the matric suction of the material, and r_{ext} and r_{int} refer to the external and internal radii of the menisci (Figure 3.2.4.1).

In this study, the surface tension for water was adopted as the physical constant for the deionized water ($T = 0.073 \text{ N/m}$). The capillary force then can be

calculated using the gorge method proposed by Hotta *et al.* (1974), by summing the water surface tension and the pressure difference on the neck of the bridge:

$$F_{cap} = S\pi r_{int}^2 + T(2\pi r_{int}) \quad (3.2.23)$$

The volume of the capillary bridge can later be calculated as an integration of the menisci profile from x_{c1} to x_{c2} , subtracting the volume of solid particles within the same area (Figure 3.2.4.1):

$$V_{cap} = \int_{x_{c1}}^{x_{c2}} \pi y^2 dx - \int_{x_{c1}}^{x_1} \pi y_1^2 dx - \int_{x_2}^{x_{c2}} \pi y_2^2 dx \quad (3.2.24)$$

where y refers to the distance between the menisci and the x axis, y_1 and y_2 are the distances between the menisci and the x axis at the liquid-particle interfaces. The iterative method developed by Wang (2014), which efficiently reproduced the capillary strengthening effect, was also adopted in this study.

3.2.4.2 Iterative method

By considering a pair of spherical particles under a constant suction condition, the internal and external radii (r_{int} and r_{ext}) of the capillary bridge can be defined when the matric suction (S), the contact angles (θ), the interparticle distance (D) and the particle radii (R_1 and R_2) are confirmed.

In DEM, the interparticle distance and the particle radii can be obtained and updated during the simulation process. The internal and external radii of the menisci then can be estimated with the imposed values of matric suction and liquid-particle contact angle. Figure 3.2.4.2 shows a pair of spherical particles (O_1 and O_2) with certain radii and a specific liquid-particle contact angle. As the meniscus of the capillary bridge is assumed as an arc of the hypothetical circle

(O_3), a capillary bridge with fixed local geometries can be produced attaching to the adjacent particles at each possible interparticle distance (Wang, 2014).

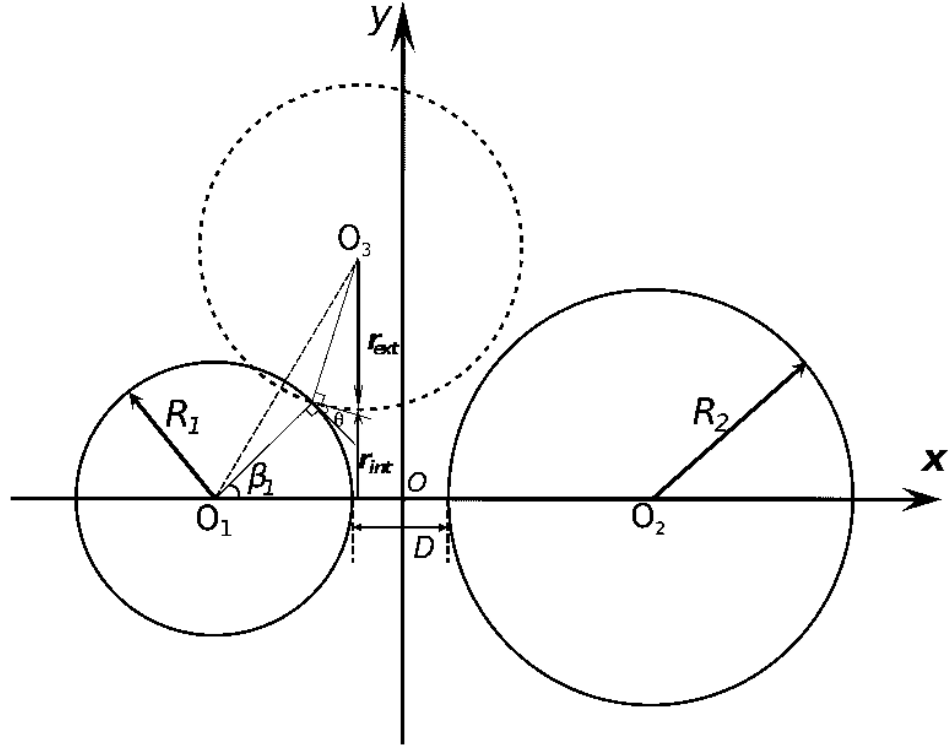


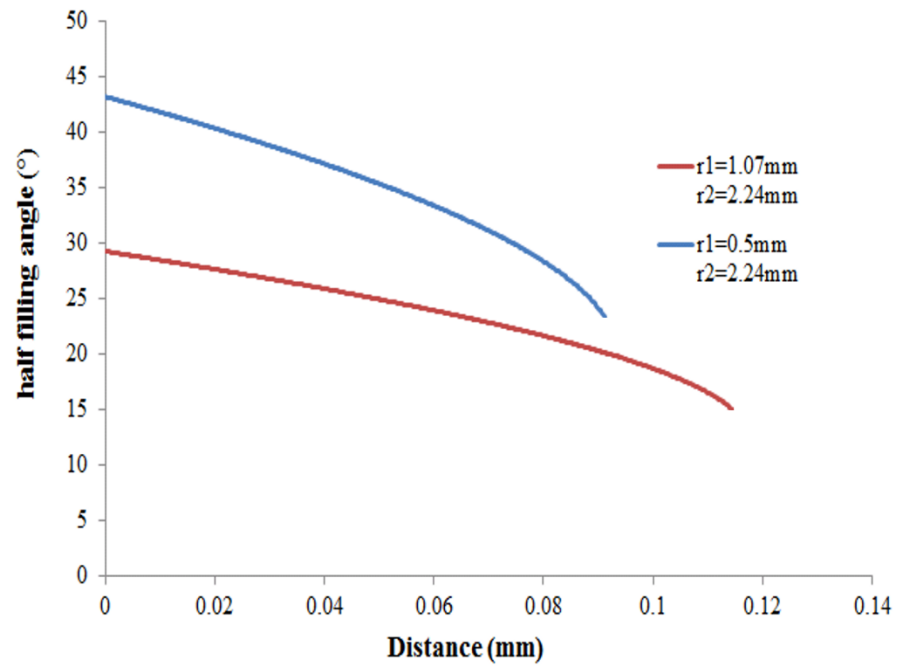
Figure 3.2.4.2 Toroidal approximation method for the estimation of capillary bridge (Wang, 2014).

The iterative method starts by suggesting a half-filling angle on particle O_1 as $\frac{\pi}{2}$. By adopting the imposed value θ as the contact angle (θ_1) on particle O_1 , calculations can be carried out to determine the position of the intersection point of the meniscus (arc) and the particle. After determining the intersection point on particle O_1 , the iterative method will try to find an applicable intersection point on particle O_2 . The half-filling angle (β_1) of particle O_1 will be decreased by $\frac{\beta_1}{2(n+1)}$ when there is no intersection point or the contact angle on particle O_2 is smaller than θ_1 , where n is the current iteration step. β_1 will be raised by $\frac{\beta_1}{2(n+1)}$ when the contact angle on particle O_2 is larger than θ_1 . Menisci with

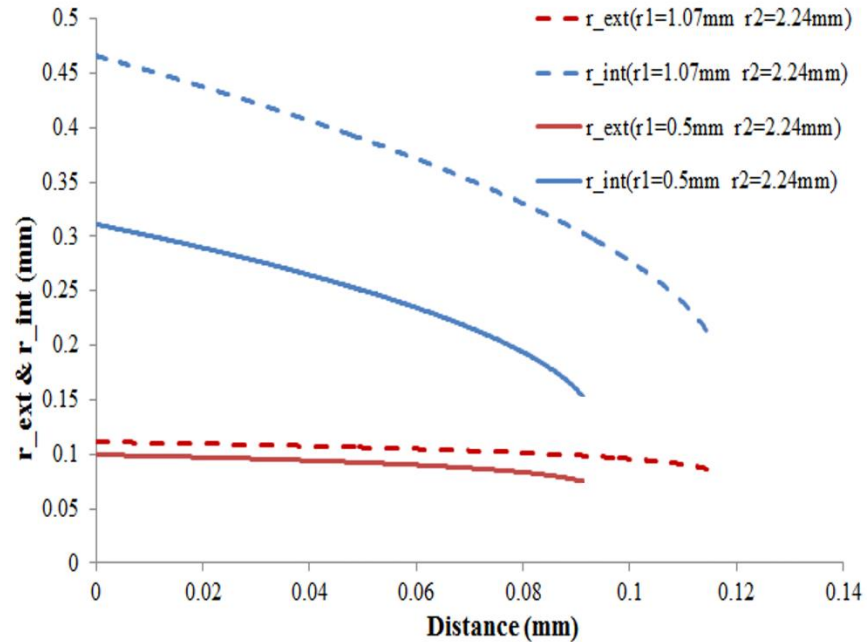
certain internal and external radii then can be obtained when the contact angle on particle O_2 meets a certain requirement. To achieve the highest capillary strengthening effect, identical contact angles ($\theta = 0$) are adopted in this study. The difference between the contact angles in a particle pair was limited to be within $\frac{\pi}{1800}$. The volume of the capillary bridge and its corresponding capillary force then can be determined by Equation 3.2.23 and Equation 3.2.24. By using this method, two sets of common solutions for the geometries of capillary bridges were determined. The evolutions of half-filling angles (β_1 and β_2), and the internal and external radii of the menisci (r_{int} and r_{ext}) were plotted in Figure 3.2.4.3.

The input parameters included the water-particle contact angle (θ), water surface tension (T) and particle radii (R_1 and R_2). It could be found from Figure 3.2.4.3a that the half-filling angle decreased gradually when two spherical particles moved apart from each other. The same phenomenon could also be found with the internal and external radii of the capillary bridge (Figure 3.2.4.3b). Note that the rupture distance $D_{rupture}$ also could be defined with the iterative method, as a solution no longer existed after the interparticle distance reached a certain limit. In these two tests, $D_{rupture}$ was determined as 0.1148mm for $R_1=1.07$ mm and $R_2=2.24$ mm, and 0.0914mm for $R_1=0.5$ mm and $R_2=2.24$ mm. The value of liquid-particle contact angle was adopted as 0 in this study, as the highest capillary force could be produced with lower value of contact angles with the iterative method (Wang, 2014). The efficiency of this model needs to be further verified in a future study as many assumptions were made. By using X-ray CT

scanning, the geometric information of a soil assembly can be obtained to further validate and modify this method.



(a) half-filling angle vs. interparticle distance



(b) external & internal radii vs. interparticle distance

Figure 3.2.4.3 The geometric information of capillary bridge estimated by the iterative method.

3.2.5 Loading Methods

3.2.5.1 Time-step in simulation

In DEM simulations, the simulation time for deformation is dependent on the amount of calculation for each time-step and the total time-step number. For sphere assemblies with similar quantities of particles, it can be assumed that they have similar numbers of calculations for each time-step. In a DEM simulation, the total amount of computation therefore is mainly dependent on the time-step. Belytschko (1983) has proposed a solution for the critical time-step in DEM simulation based on the natural frequency of a spring-mass oscillation system. It has been proved as a stable method in different previous research (Richefeu *et al.*, 2007; Scholtès *et al.*, 2007; Feng *et al.*, 2002). In this solution, the time-step for Hooke's contact model is determined by:

$$\Delta t = \sqrt{\frac{m}{k_n}} \quad (3.2.29)$$

where m refers to the mass of the particle, and k_n is the contact stiffness. In Hertz contact model, the contact stiffness can be determined as $k_n = \xi E^* R$, where ξ is a constant and R is the particle radius. The mass of the particle then can be calculated from the particle density (ρ) and particle size:

$$\Delta t = \sqrt{\frac{m}{k_n}} = \sqrt{\frac{\rho R^3}{\xi E^* R}} = R \sqrt{\frac{\rho}{\xi E^*}} \quad (3.2.30)$$

It can be concluded that for particle assemblies with the same elastic property and particle density, the value of a single time-step is in accordance with the size of particles. For assemblies with larger particle size, the increase in the time-step is proportional to the increase in particle size. For two systems with identical deformation rate, the same value of total time-steps can be used to achieve a

similar strain state in the RVEs. Therefore, the total simulation time, as a determinate value is highly independent of the mean particle size.

3.2.5.2 Servo-control for boundary walls

New micro-mechanical properties were introduced in the model after the preparation stage. The triaxial test was simulated by confining the spherical particles using six smooth walls under gravity-free conditions. Note that all walls were defined as frictionless in order to avoid any friction between particles and the loading platens, therefore allowing the applied stresses to remain normal to each wall. A servo control system was implemented on the boundary walls, assuming each boundary as a servo wall that is able to compact the specimen until a total target force is reached. The target force of the servo boundaries can be calculated from the confining pressure with the changing strain values in each time step. Thus:

$$F_{t,1} = \sigma_2 l_{x,1} l_{z,1} \quad (3.2.27)$$

where $F_{t,1}$ is the newly updated target force after every time step, which depends on the constant confining stress σ_2 and the current length of the specimen $l_{x,1}$ and $l_{z,1}$. Displacements of the lateral walls were thus able to remain at a constant value of confining stress. During the triaxial loading, the top and bottom walls moved vertically to increase the loading, while the lateral boundaries were maintained at the confining pressure. The axial strain can be calculated as:

$$\varepsilon_1 = \frac{l_1^0 - l_1}{l_1^0} \quad (3.2.31)$$

$$q = \sigma_1 - \sigma_2 \quad (3.2.32)$$

where l_1 denotes the current specimen length in the axial direction and l_1^0 is the initial axial length. σ_1 and σ_2 stand for the major and minor principal stresses respectively.

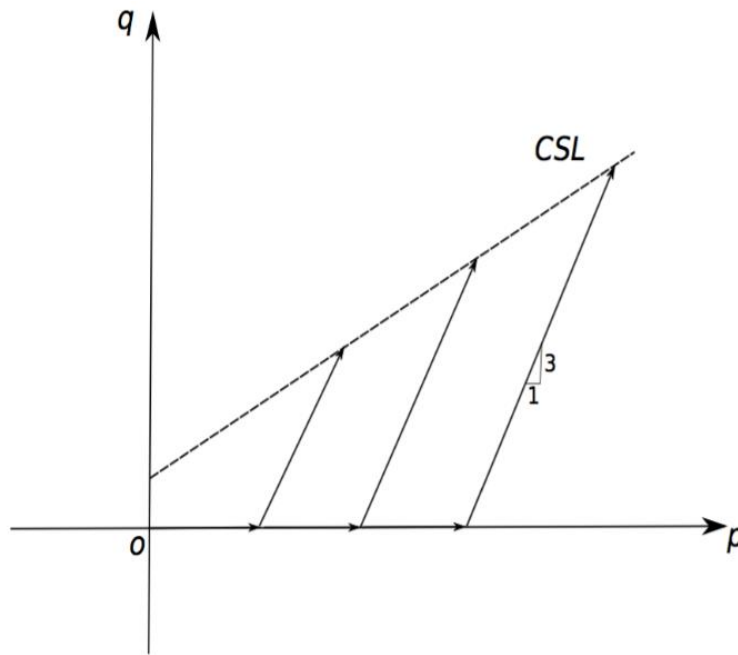


Figure 3.2.5.1 Sketch paths of isotropic compression and triaxial shearing ([Wang, 2014](#)).

Moreover, Figure 3.2.5.1 illustrates the typical paths of isotropic compression and triaxial shearing ([Wang, 2014](#)). The sample system was firstly consolidated from a very low stress condition under isotropic compression. After being isotopically compressed to different states of confining pressure, the sample was then sheared by a triaxial compression test. In this study, the sample pack was firstly confined in a stress-controlled mode by specifying the target stress and the maximum velocities allowed at the surrounding walls. The triaxial loading was then conducted under a strain-controlled condition by defining the maximum velocities of the top and bottom walls. According to the simulation

results, the stress and strain states within the specimen can be assumed as homogeneous. The wall stresses then can be directly obtained from the boundary conditions, and the corresponding strains can be calculated from wall displacements.

3.2.5.2 Control of unbalanced force

To avoid dynamic effects during DEM simulation, the quasi-static equilibrium is maintained after the calculation of each time step. The unbalanced forces in the system are controlled within a certain condition to achieve an approximate quasi-static condition. The unbalanced ratio applied to quantify the quasi-static equilibrium is defined by:

$$U = \frac{F_{UB}}{F_C} \quad (3.2.32)$$

where F_{UB} refers to the mean unbalanced force on the particles in the assembly. F_C is defined as the mean contact force over all the contact points on particles. In this project, the isotropic and triaxial compressions are assumed as quasi-static when the unbalance ratio was less than 0.01. If the limit is exceeded, the boundaries will be suspended for a certain number of time-steps until the unbalanced ratio is decreased to satisfy the quasi-static equilibrium.

3.3 X-ray Computed Tomography

3.3.1 Basic Features

The mechanical behaviour of unsaturated granular soils is significantly dependent upon the soil microstructure which includes shape, arrangement and distribution of particles, liquid and void space within a soil material. With X-ray

CT scanning, a digital image can be created by measuring the X-ray linear attenuation coefficient of an object, which is dependent on the density of a material (Nielsen, 2004). Materials with different densities will present a different appearance under X-ray CT scanning. Normally a high density-material will attenuate more X-rays than a material with lower density. During the past decade, a number of studies have been conducted to measure soil properties at microscale, including void ratio, physical density, particle size distribution, *etc.* (Tollner *et al.*, 1998; Nielsen, 2004). These have proven some capabilities and advantages of X-ray CT in measuring the soil microstructure. Its application in geotechnical engineering is still at an early stage, however the rapidly developing technology has driven more researchers to study and investigate in this area.

Compared to traditional methods, the major advantages of X-ray CT include minimal sample disturbance and time savings. A study by Tollner (1998) showed that X-ray scanning can provide particle size data consistent with the conventional methods but without the time-consuming preparation process. Due to the minimal disturbance during the scanning, X-ray CT also allows the granular sample to be scanned multiple times. This superiority makes it possible for the investigation of particle and pore interactions at any time and locations within a soil sample. In this study, a cylindrical container with spherical glass beads will be scanned and studied using the X-ray CT technique. This method will be used to determine the geometry and the spatial distribution of capillary bridges within a granular assembly. These features then will be implemented into the DEM model.

3.3.2 Apparatus

Figure 3.3.2.1a shows the pycnometer used in this study. During the sample preparation, the particle density of glass beads in each specimen was firstly determined using the pycnometer. An analytical balance with an accuracy of $1 \times 10^{-4}g$ was adopted for all measurements (Figure 3.3.2.1b). A syringe with a volume of $1ml$ was used to measure the deionized water required. To avoid diffusion in X-ray CT and achieve better resolution, polypropylene was used to manufacture both the tube and the caps of the test tube (Figure 3.3.2.2). Caps with the same specifications were used to seal both ends of the test tube.

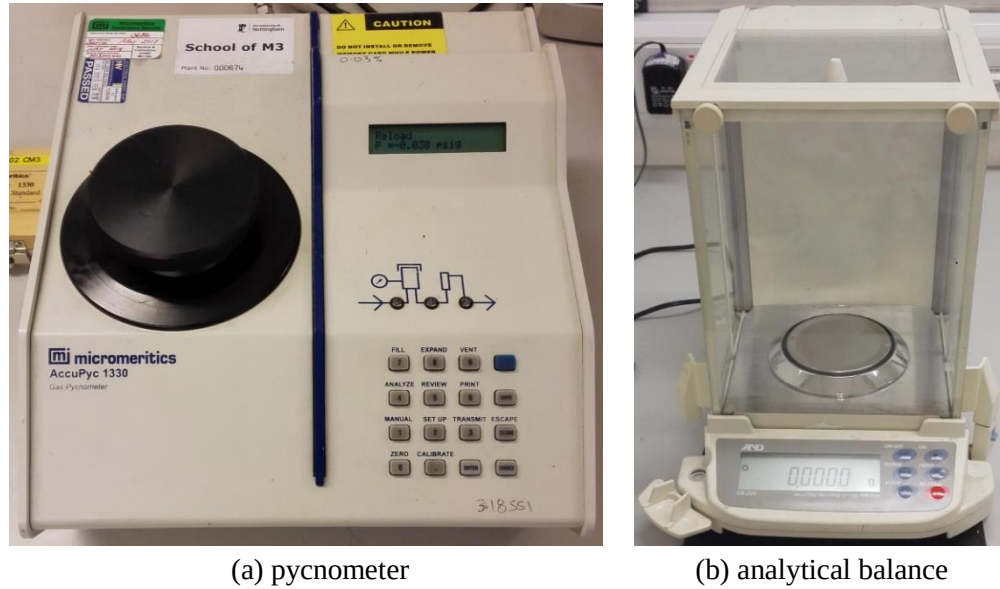


Figure 3.3.2.1 Apparatus used for the preparation of experimental specimens.

The specifications of the test tube are also illustrated in Figure 3.3.2.2. As the length of the stopper on the cap was 10mm, the applicable volume of the test tube (V_t) could be calculated as:

$$V_t = \pi r_c^2 l_t = \pi \times 0.004^2 \times 0.03 = 1.508 \times 10^{-6} m^3 \quad (3.3.1)$$

where r_c refers to the radius of the cylindrical stopper attached to the cap, l_t stands for the applicable length of the cylindrical tube for loading glass beads.

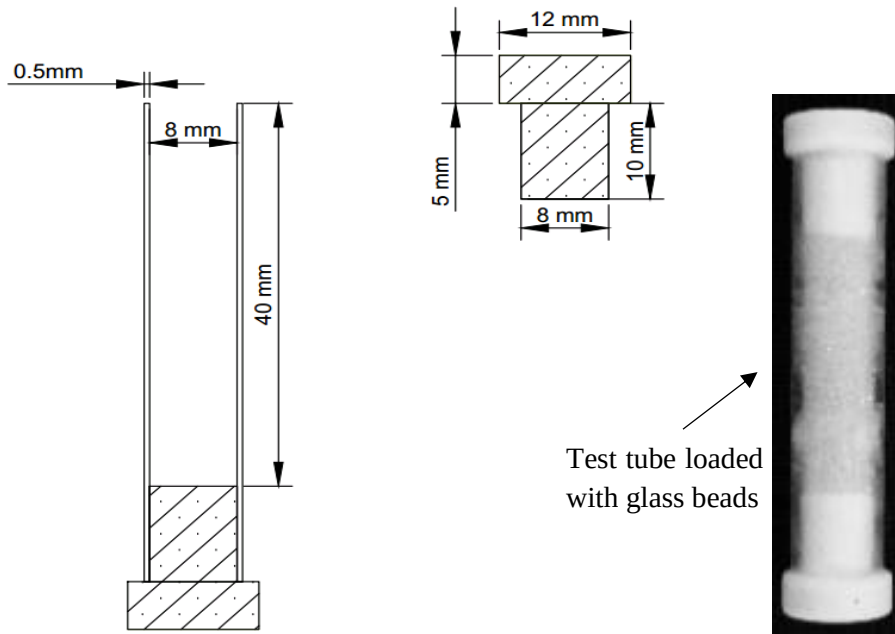


Figure 3.3.2.2 Specifications of the test tube.

3.3.3 Sample Preparation

Firstly, calibration was carried out for the pycnometer according to the instruction (Figure 3.4.1a). The practical particle density of the glass beads in use was then determined using the pycnometer. The weight of the test tube with both caps (W_w) was later determined using an analytical balance. With a specific value of the imposed porosity ($n = 0.43$) and the applicable volume of the test tube ($V_t = 1.508 \times 10^{-6} m^3$), the total volume of glass beads (V_s) and the volume of the pore space (V_a) were calculated respectively:

$$V_s = V_t \times (1 - n) \quad (3.3.2)$$

$$V_a = V_h \times n \quad (3.3.3)$$

The weight of the glass beads thus could be calculated using the particle density estimated previously:

$$W_s = M_s g = V_s \rho_d g \quad (3.3.4)$$

Glass beads with the same weight were then collected on a polypropylene plate and determined using the analytical balance.

To produce a sample specimen with an imposed saturation degree (Sr_t), the volume of required water was calculated using the volume of pore space determined previously ($V_w = V_a Sr_t$). Deionized water was then slowly injected onto the glass beads pile on the polypropylene plate with the syringe, until the required weight of water was achieved ($W_w = V_w \rho_w g$). A steel rod was used to mix the water with glass beads to achieve the maximum level of uniform distribution. To avoid the evaporation of water, the mixing time in this study was limited to be within 60 seconds. The glass beads and the water were then loaded into the test tube after the mixing process. The total weight of the test tube with the glass beads and water (W_{w1}) was determined using the analytical balance. As it was assumed that the weight of air could be neglected in this study, the weight of the imposed water (W_θ) thus could be calculated by:

$$W_\theta = W_{w1} - W_w - W_s \quad (3.3.5)$$

From the mass of the imposed water, the actual saturation degree (Sr_p) could be calculated for the sample specimen. The steps above were repeated three times to produced three sample specimens with a series of imposed saturation degrees ($Sr_t=6\%$, 9% and 12%).

3.3.4 Setup for X-ray Computed Tomography

3.3.4.1 XRADIA Versa XRM-500

XRADIA Versa XRM-500 microscopy can provide 3D X-ray imaging with submicron resolution (Figure 3.3.4.1). Non-destructive observation of the internal structure of materials can be achieved with the Versa XRM-500. X-ray images of a sample specimen can be captured and restored into a 3D volume using computer analysis. Multiple cross-sections can be acquired in the plane under scan.

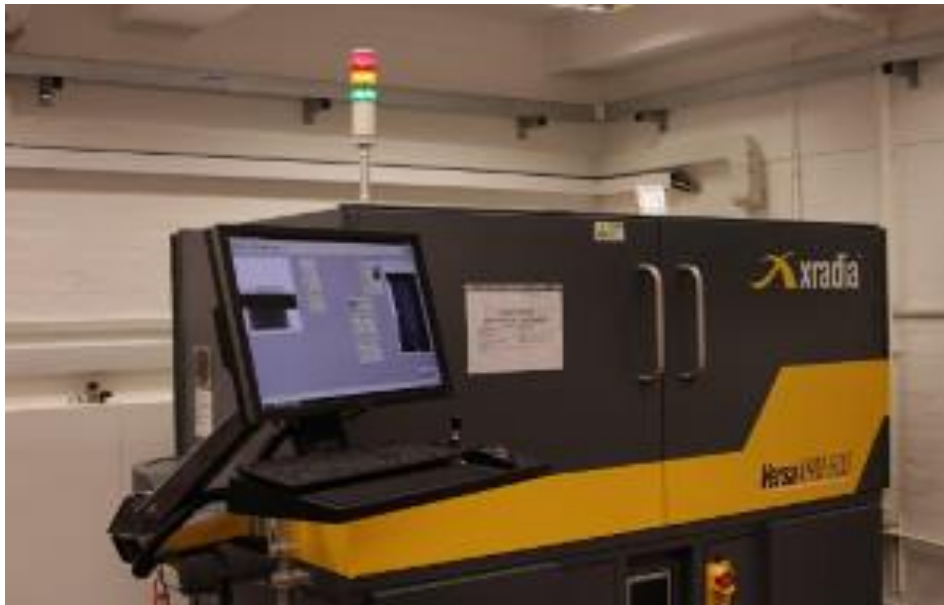


Figure 3.3.4.1 XRADIA Versa XRM-500.

The Versa XRM employs a series of objectives allowing variable magnification. It enhances the selection of magnification by changing objectives or the geometric information. While conventional microCT and nanoCT systems are usually limited to only geometric magnification, the Versa XRM facilitates the operation over resolution and phase contrast across a vast range of sample sizes and a large working distance. Thus, it can be applied to a wide range of subjects, including semiconductors, material science, geology and life sciences.

3.3.4.2 X-ray CT scanning process

The test tube was attached to the sample holder and then secured on the sample stage in the X-ray CT facility. The axis of the sample stage was firstly recalibrated, and other operating parameters, such as voltage and power were adjusted. The mode of tomography was used to produce image slices which would be used for 3D reconstruction later. The position of the sample stage was then adjusted to manipulate the sample into the path of the x-ray beam line. The x-ray source and the detector were moved to the positions needed to confirm that they would not collide with the sample in a full rotation of plus or minus 90°. The X-ray source was then activated after closing the door of the facility. The sample was moved to the desired position, with rotation axis configured as in the z direction. To produce images with the desired quality, other scanning parameters were adjusted, including the exposure time, readout time, starting angle, end angle, and number of images requested. Figure 3.3.4.3 presented all scanning parameters adopted in this study.

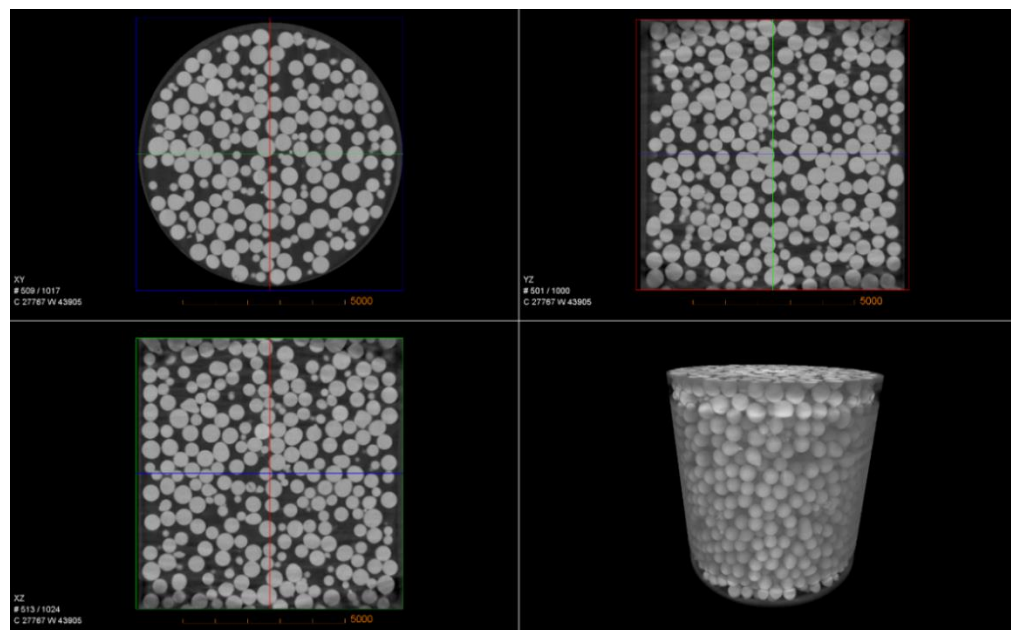


Figure 3.3.4.2 2D cross-sections and 3D reconstruction of the scanned specimen.

The TXM Reconstructor program was then used to assemble the acquired images into an accessible format. Several corrections, such as final center shift and beam correction could be made to the images if necessary. TXM 3D Viewer was used to view the volume and cross-sectioned slices. After reconstruction was completed, the image could be viewed in TXM 3D Viewer. Figure 3.3.4.2 showed the images presented in TXM 3D Viewer, with 2D cross-sections in each plan, 3D reconstruction of the scanned volume.

Imaging Mode:	Tomography	Source Information	
Camera Binning:	2	Power:	6.04
Camera Temperature:	-59 C	Voltage:	70.08
File Data Type:	USHORT	Target Current:	86.25
Display Data Type:	FLOAT	Tube Current:	183.51
Image Size:	1024 x 1024	Centering X:	-101.03
File Size:	3200.000 MB	Centering Y:	13.63
Source Filter:	LE2	Vacuum Level:	2.08
Source Setting:	70 kV 86 uA	Focus Current:	1495.10
Source-RA distance:	16.2995 mm	Hours on target:	13.45
Detector-RA distance:	116.6956 mm	Target turn #:	126
Pixel size:	8.2742 um	Filament:	1.572
Optical Magnification:	0.39992 (0.4X)	Cold Cathode Status:	On
Exposure Time:	1.2000 sec		
Camera Readout:	Fast (2.5 MHz)		
Heated Sample Temp:	NA		
Date and Time:	12/15/16 10:47:07		
Frames/Image:	NA		
Exp/Frame:	NA		

Figure 3.3.4.3 Scanning parameters adopted in X-ray CT.

3.3.5 Image Process

3.3.5.1 Noise filtering and pre-process

The cross-sections from the top and bottom of the sample specimens were firstly removed to eliminate the artifacts from the X-ray CT. Figure 3.3.5.1a shows an example of the discarded images slices, where blurred water phase could be

observed. A total number of 600 image slices, located at the center of the sample specimen, were eventually adopted in the image processing (Figure 3.3.5.1b). The median filter in Avizo is a nonlinear digital filtering technique that preserves edges. It can be adopted to reduce the scatter dots in the grayscale images, and to accomplish better accuracy in the calculation of size distribution. A median filter with 3D interpretation was applied to the remaining image stack as a noise reduction method. Grayscale normalization was also conducted prior to the segmentation process.

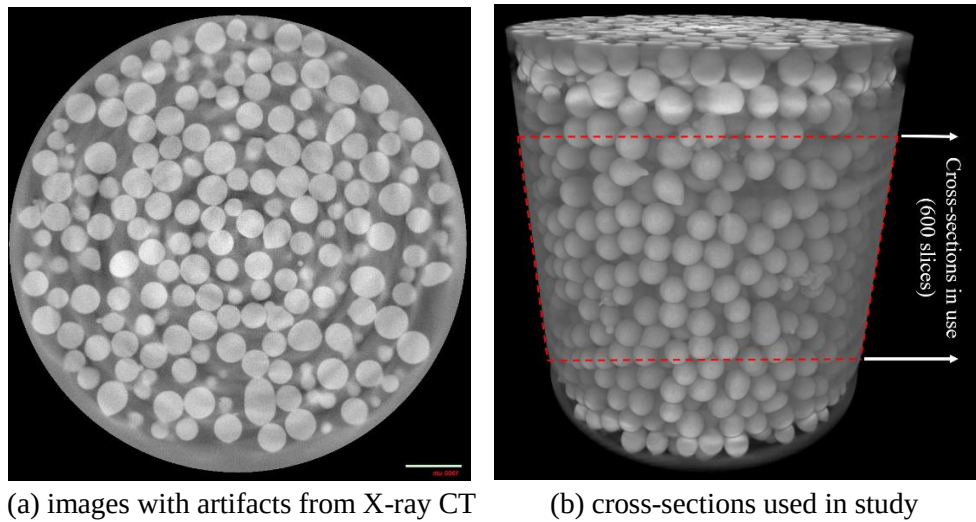


Figure 3.3.5.1 Region of interest in image processing.

3.3.5.2 Segmentation of three phases

Segmentation of three phases (air, water and particle) was carried out after conducting the noise filtering. As a simple technique requiring less manual interaction, threshold segmentation was applied based on the gray values of the image data. The water phase in the images was firstly segmented by adjusting the minimum and maximum thresholding values to 82.12 and 101.57 respectively. The water phase was then segmented using values from 40 to 82.12. By applying thresholding values from 101.57 to 300, the particle phase was

segmented last. Binary images of the three phases were produced for each unsaturated specimen by repeating the procedures with the same thresholding values. Material properties including porosity and saturation degree were determined by calculating the corresponding volumes in the binary image.

3.3.5.3 Analysis of particle size distribution

By simulating the flooding from a series of labelled objects in the 2D image, the watershed algorithm in Avizo can expand regions according to a priority map until the watershed lines are approached ([Visualization Sciences Group, 2013](#)). As an efficient method for automated object segmentation, this method was applied in this study for particle separation.

The binary images of the particle phase were acquired after carrying out the threshold segmentation. To proceed particle separation, the Chamfer Distance Map module was firstly attached to the binary image using the 3D interpretation. Secondly, the H-Maxima module was applied using a contrast value of 4, to produce binary images consisting of the merged maximum values of the contrast variation from the input distance map. The module Labeling was then applied to the binary images to create markers for individual maximum region. Since the markers in the watershed algorithm will expand towards the higher values of the input priority map, a Not module was later applied to the distance map for image inversion. Images of watershed separation lines were then produced by attaching a Marker-Based Watershed module to the images with the reversed distance map. The separation lines could be extracted from the binary images of particles, using

the AND NOT Image module. By repeating the procedure above, binary images of separated particles were generated for each unsaturated specimen.

To calculate the number of particles in the plane of interest, the module Labeling was later applied to the binary images containing separated particles. The volume of each labelled particle was determined using the module Label Analysis. The particle size distribution of each unsaturated specimen was evaluated and is plotted in chapter 5.

CHAPTER 4: Triaxial Test Simulations of Unsaturated Granular Materials

4.1 Introduction

In unsaturated soils subjected to capillary effects, the presence of water could lead to the formation of capillary bridges between neighboring particles, introducing new interparticle forces. For granular materials commonly composed of distinct particles, specific interparticle interactions could be significantly influential on their macroscopic behaviour. As a pertinent approach, particle scale modelling could be adopted for unsaturated granular soils correlating physical fundamentals to locally induced effects.

To validate the three-dimensional discrete element method (DEM) in modelling the mechanical behaviour of granular materials, a numerical assembly was firstly generated to reproduce the mechanical behaviour of dry granulates under triaxial compression at the macroscopic scale. Figure 3.2.5.1 demonstrates a common loading path of the triaxial compression test. The deviatoric stress could be expressed as the difference between the major and minor principle stresses. The quasi-static condition was maintained during triaxial compression by introducing the unbalanced force ratio. By adjusting the axial strain rate, the unbalanced ratio was controlled to be less than 0.01 in this study. Since only spherical particles were used in this study, rolling resistance was adopted between contacting particles for dry assemblies. Four principal input parameters were investigated at micro-scale, including the normal and tangential contact

stiffness, friction coefficient and coefficient of rolling resistance. According to the previous laboratory results on the Labenne sand, which had a similar grading curve to LB sand ([Belheine, 2008](#)), a set of dry triaxial test simulations were carried out to calibrate the macroscopic responses of the numerical particles.

For unsaturated granular materials in pendular states, where water is under the form of capillary bridges between particles, the toroidal approximation method allows the force induced by these bridges to be linked to the local geometry of the particles and to the matric suction acting in the soil. DEM simulations were then conducted using spherical particles with capillary bridges estimated by the toroidal approximation. It was assumed that capillary bridges could be simplified as toroidal shapes and the matric suction between particles was maintained to be constant during every test. According to the SWCCs produced by Wang ([2014](#)) using the same capillary bridge model, the hydraulic property of the unsaturated material could be efficiently replicated using the toroidal approximation method. Triaxial compression tests were later conducted using the unsaturated assemblies with uniform water distribution until the critical state was achieved. The macroscopic behaviour of unsaturated materials was presented, including deformation mechanism, critical state and deviatoric stress paths. The evolution of saturation degree along the axial strain was also investigated. The same matric suction (20kPa) and void ratios ($e=0.629$ and 0.733) were adopted in the numerical assemblies with uniform water distribution. To investigate the influence of the spatial distribution of capillary bridges, different distribution models for capillary bridges were later introduced. Capillary bridges were only permissible with certain volume fractions (25% and 75%) of each distribution

model. The macroscopic behaviour of various distribution models under triaxial compression tests is also presented in this chapter. Finally, triaxial test simulations were carried out using two numerical assemblies with identical initial saturation degrees but different water volume fractions. The influence of particle size on capillary effect was also analysed.

4.2 Calibration with Dry Granular Materials

4.2.1 Numerical Assembly

The numerical sample used in the triaxial test simulation was a cubic assembly (Figure 4.2.1.1). The sand particles were modelled with spheres, using the Hertz-Mindlin contact model. The particles were given a Poisson's ratio (ν) of 0.25, a density (ρ) of 2500kg/m^3 and a Young's modulus E of 70GPa . The same parameters were adopted as those used in the previous research by Wang (2014).

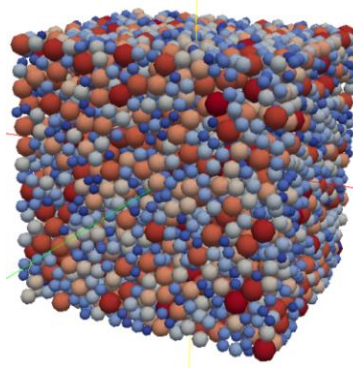


Figure 4.2.1.1 Numerical specimen in dry triaxial test simulations.

For calibration purpose, a grading curve similar to Leighton Buzzard (LB) sand fraction E was firstly used for the numerical specimen. Figure 4.2.1.2 shows the particle size distribution (PSD) curves of both the LB sand and the spherical particles in the calibration tests. For validation, dry triaxial tests were conducted to compare with the experimental data from previous publication proposed by

Belheine *et al.* (2008). All numerical assemblies contained more than 9000 particles and were generated using the radius expansion method. For a collision between two particles, the restitution coefficient is defined as the ratio of the relative velocity after to the relative velocity before the collision. It was configured to be 0.2 in this study.

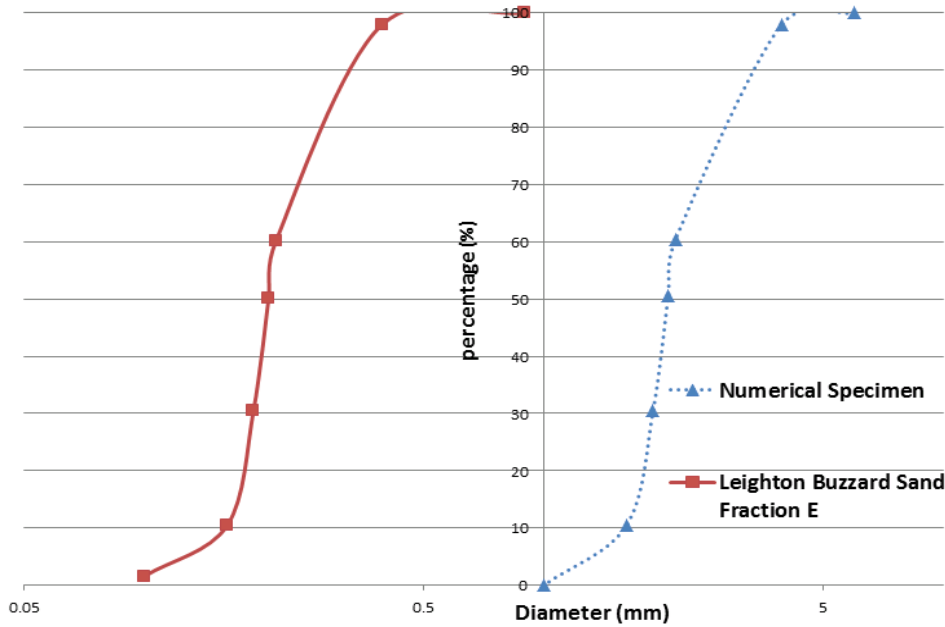


Figure 4.2.1.2 Particle size distribution of LB sand fraction E, and numerical specimen in dry triaxial test.

4.2.2 Calibration with Dry Material

4.2.2.1 Microscopic parameters

During the stage of calibration, the microscopic parameters that were adopted in the DEM model were adjusted by comparing the numerical results with the experimental ones. It was found that some parameters have cross effect on the macroscopic behaviour. For example, the coefficient of rolling friction μ_r and the angle of interparticle friction β could both affect the peak deviatoric stress (Figure 4.2.2.1). A series of tests were carried out for calibration purposes. The

values for normal contact stiffness k_n and shear contact stiffness k_s were initially adopted according to previous studies (Liu and Sun, 2002). Values of these two parameters then were varied to investigate their effects at the macro-scale. It was noted that k_n and k_s , and their ratio $\frac{k_s}{k_n}$ could significantly affect the deformation characteristics of a granular assembly (Figure 4.2.2.2). k_n was also found to be influential on the initial gradient of the stress-strain relation curve. Furthermore, it was also found that the dilatancy angle was related to the Young's modulus. With the same specimen, a series of simulation tests were conducted to determine the appropriate local elastic parameters. While other parameters were kept constant, the angle of interparticle friction β was adjusted to validate the dilatancy curve of the real sample. After adjusting the angle of interparticle friction, the coefficient of rolling friction μ_r and the coefficient of plastic moment η_r were varied to match the stress-strain relationship to the experimental results. It was found that μ_r mainly modifies the peak stress value.

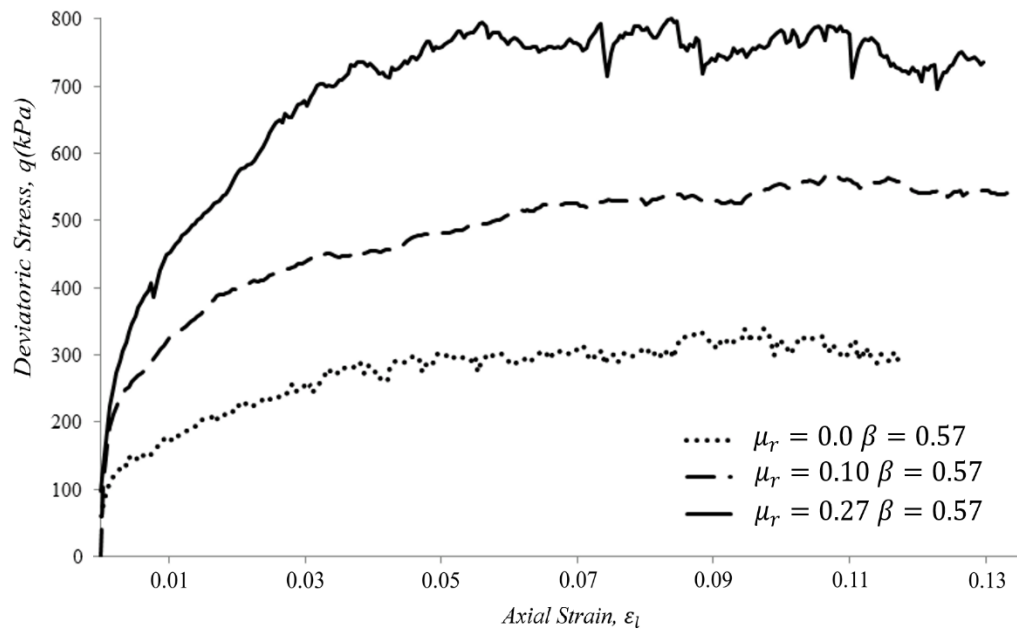


Figure 4.2.2.1 Evolution of deviatoric stress in calibration tests, with different values of rolling resistance coefficient.

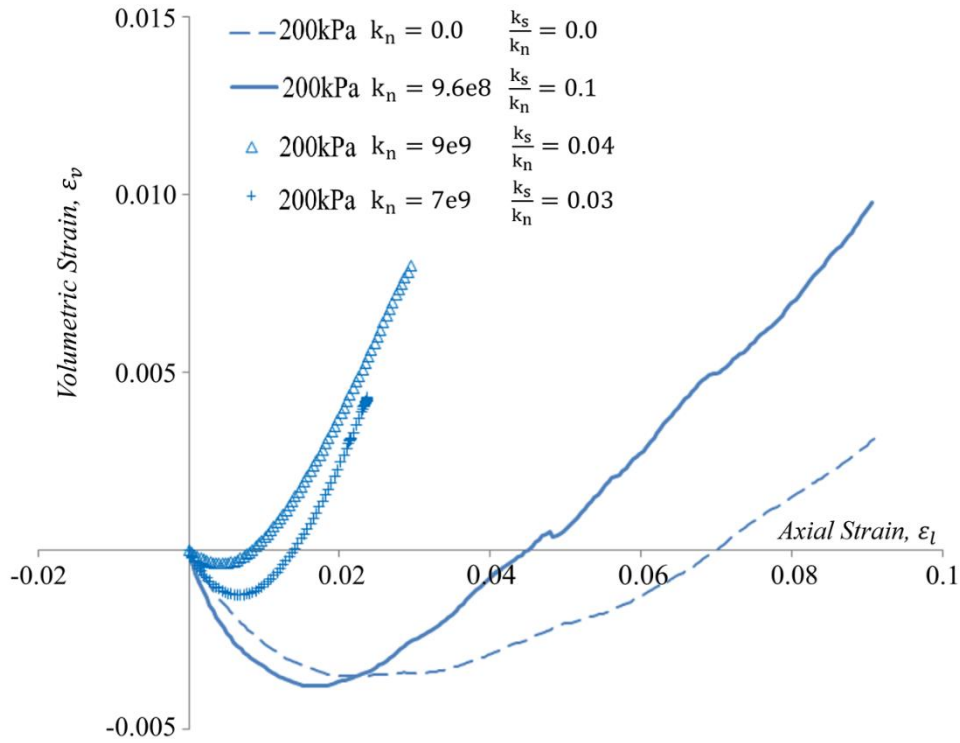


Figure 4.2.2.2 Evolution of volumetric strain in calibration tests, with different contact stiffnesses.

4.2.2.2 Modelling results

To understand the micro parameters more comprehensively, several simulation tests were carried out using the same values adopted in previous research. A Young's modulus (E) of 70 GPa was used in this model. Table 4.2.2.1 lists other microscopic parameters adopted in a study by Belheine *et al.* (2008). Figure 4.2.2.3 and Figure 4.2.2.4 show the deviatoric stress and volume strain versus axial strain for the numerical sample using these input parameters. Mohr circles are also presented as an acceptable result of the calibration procedure (Figure 4.2.2.5). The failure envelope was linear for the chosen parameters for peak and residual stresses. Since no local cohesion was adopted in this model, the failure envelope passes through the origin. It proves the ability of the modified DEM model to reproduce the macroscopic Mohr-Coulomb criterion. The slope of the

failure envelope gives a maximum macroscopic friction angle of 34.3° which corresponds to a microscopic friction angle of 30° .

Table 4.2.2.1 Input parameters tested in the calibration procedure.

	Particle-Particle	Particle-Boundary
Normal stiffness (N/m)	9.6×10^8	1.92×10^9
Shear stiffness (N/m)	3.84×10^7	7.68×10^7
Normal damping (Ns/m)	7.9×10^4	1.1×10^5
Shear damping (Ns/m)	1.4×10^4	2.0×10^4
Interparticle friction angle (deg)	30	0
Coefficient of viscous damping	1.0	1.0
Coefficient of rolling friction	0.14	0

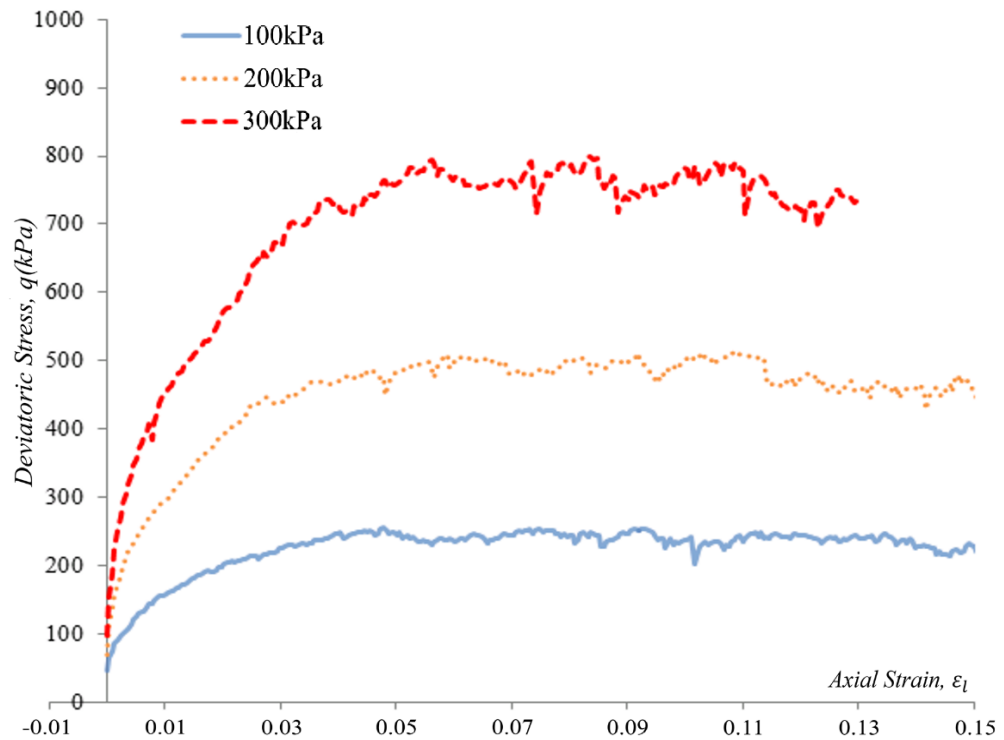


Figure 4.2.2.3 Evolution of deviatoric stress in dry triaxial tests with different confining stresses.

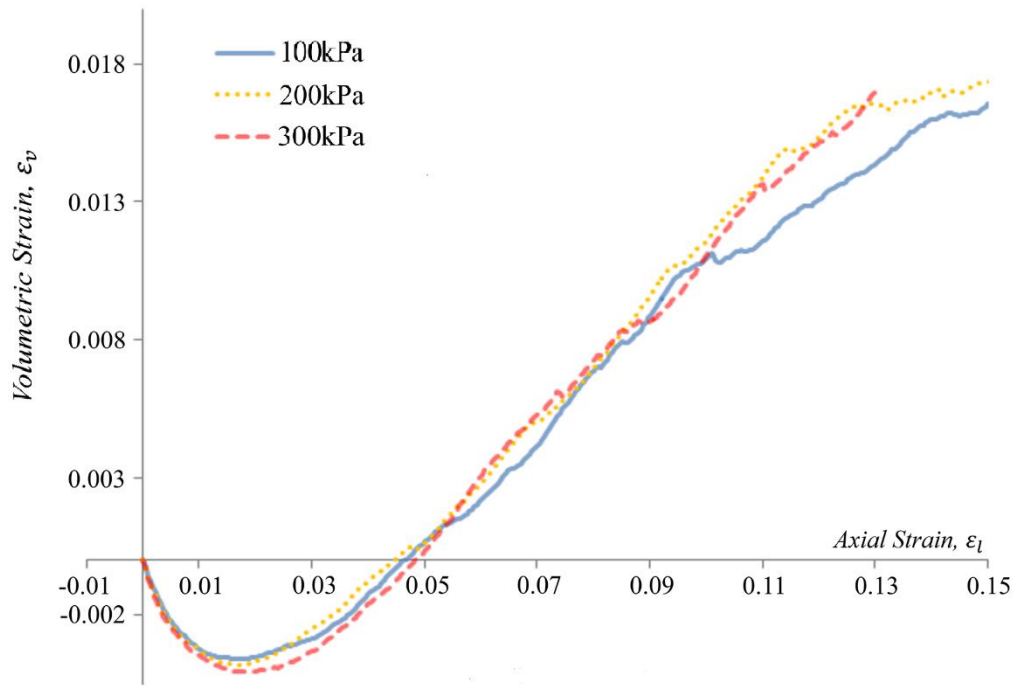


Figure 4.2.2.4 Evolution of volumetric strain in dry triaxial tests with different confining stresses.

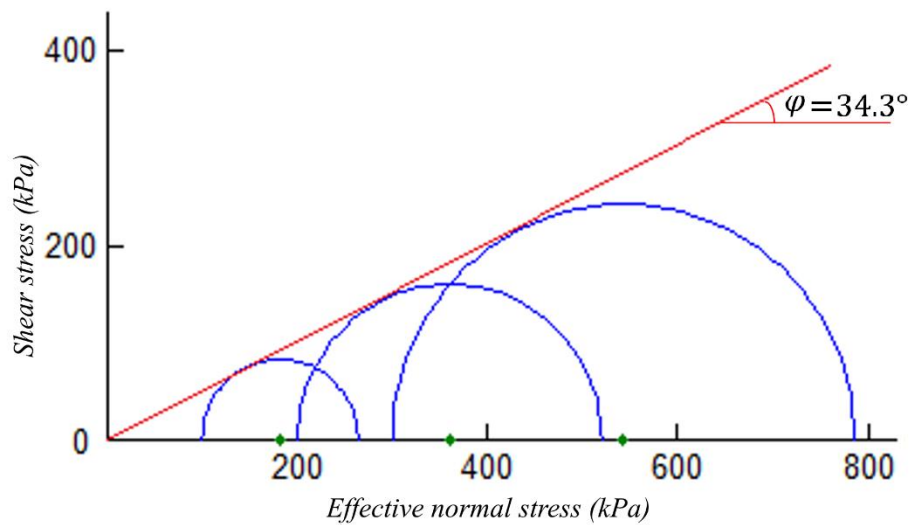


Figure 4.2.2.5 Mohr circle representation of the numerical particles according to the results of triaxial tests.

Belheine *et al.* (2008) presented a series of results of experimental triaxial tests using Labenne sand which had a similar grading curve to LB sand fraction E (Figure 4.2.2.6).

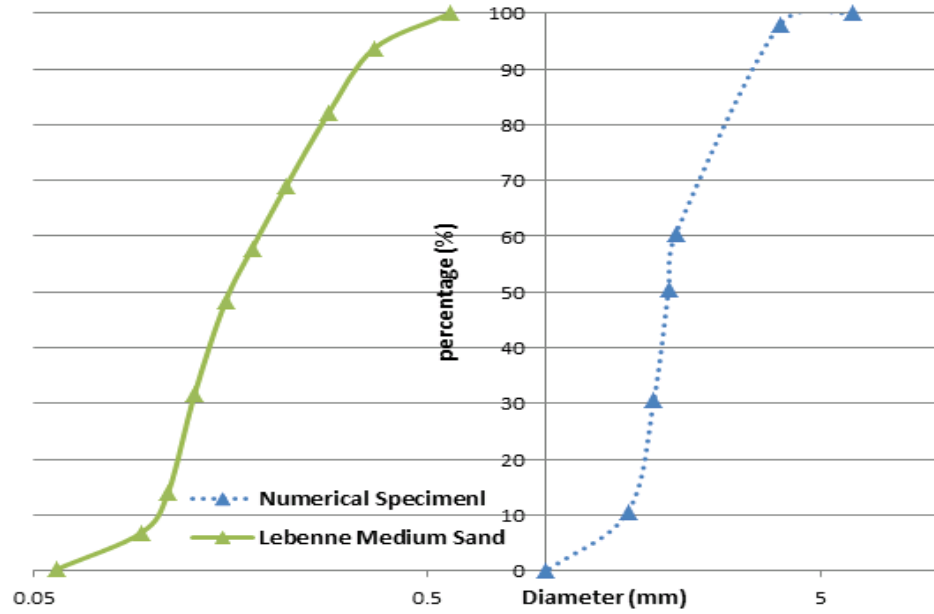


Figure 4.2.2.6 Size distribution of Labenne medium sand and numerical specimen.

Table 4.2.2.2 Input parameters used to match the experimental results.

	Particle-Particle	Particle-Boundary
Normal stiffness (N/m)	3.6×10^{10}	7.2×10^{10}
Shear stiffness (N/m)	1.44×10^9	2.88×10^9
Normal damping (Ns/m)	7.9×10^4	1.1×10^5
Shear damping (Ns/m)	1.4×10^4	2.0×10^4
Inter-particle friction angle (deg)	35	0
Coefficient of rolling resistance	0.24	0
Coefficient of viscous damping	1.0	

In this study, a series of triaxial tests with the same numerical specimen were carried out to compare with the experimental results. Microscopic parameters used in the simulation are listed in Table 4.2.2.2 and, were calibrated to match the laboratory tests (Belheine *et al.*, 2008). As for the dry assembly adopted previously, a Poisson's ratio ν of 0.25, a density ρ of 2650 kg/m^3 and an initial porosity n of 0.4 were used here. Note that a value of Young's Modulus E of 300MPa was used in this model. Different confining stresses were also adopted

(100kPa and 200kPa). Figures 4.2.2.7 to Figure 4.2.2.9 show the modelling results compared to the experimental ones.

In Figure 4.2.2.8 and Figure 4.2.2.10, very similar deformation curves could be observed between numerical specimens and laboratory granular material. However, a difference was found between the stress-strain curves. A difference was also found between the maximum values of deviatoric stresses (Figure 4.2.2.7 and Figure 4.2.2.9). The disparity might result from the relatively small quantity of particles in the numerical assembly, the small specimen size and the larger particle size.

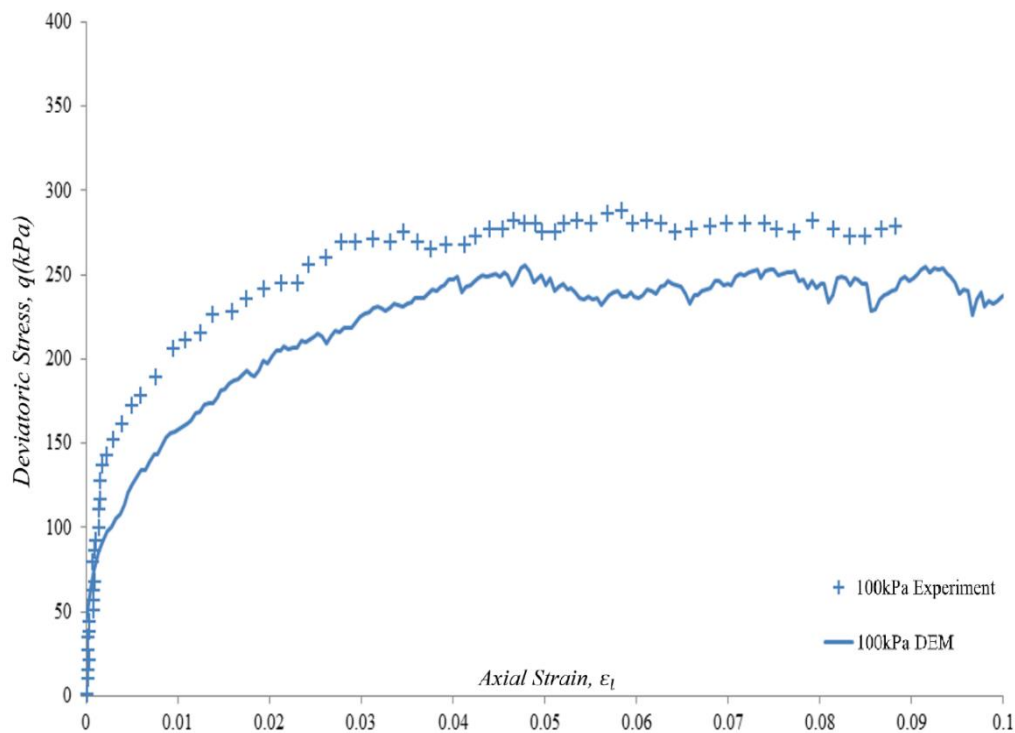


Figure 4.2.2.7 Dry specimen under triaxial compression, plotted with the experimental result, deviatoric stress vs. axial strain, confining stress=100 kPa.

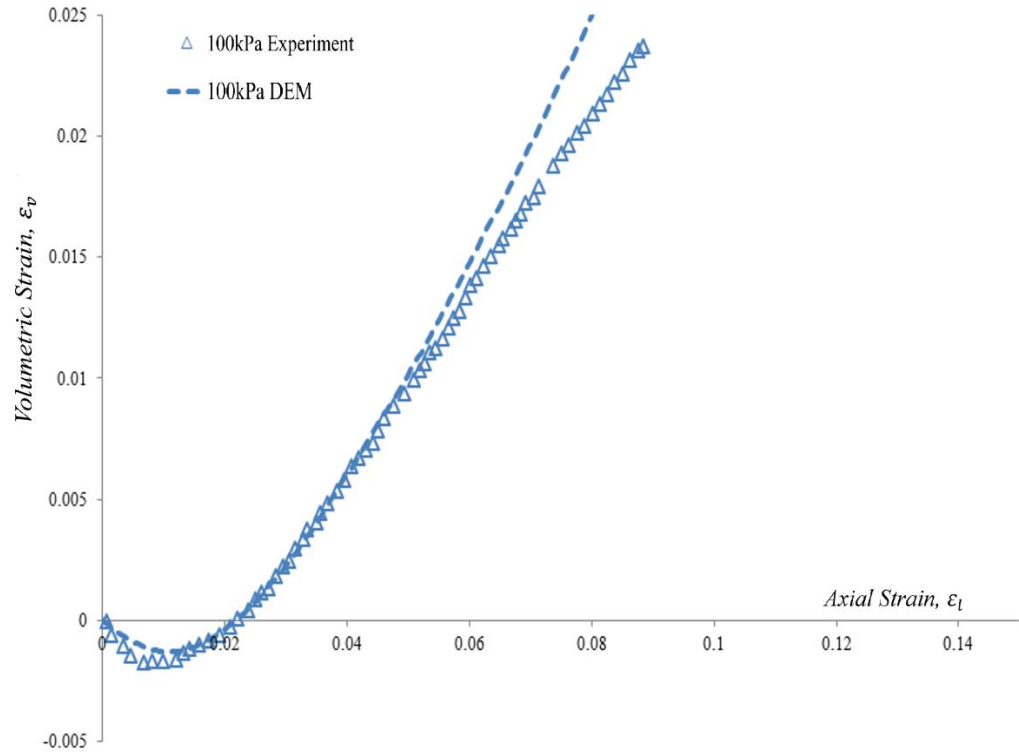


Figure 4.2.2.8 Dry specimen under triaxial compression, plotted with the experimental result, volumetric strain vs. axial strain, confining stress=100 kPa.

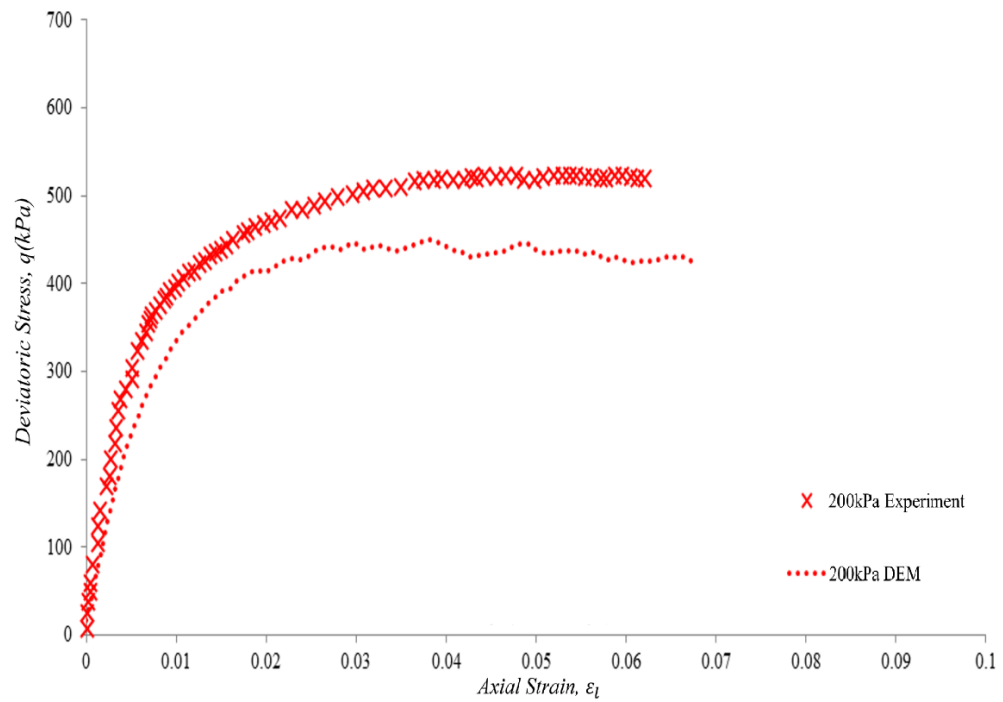


Figure 4.2.2.9 Dry specimen under triaxial compression, plotted with the experimental result, deviatoric stress vs. axial strain, confining stress=200 kPa.

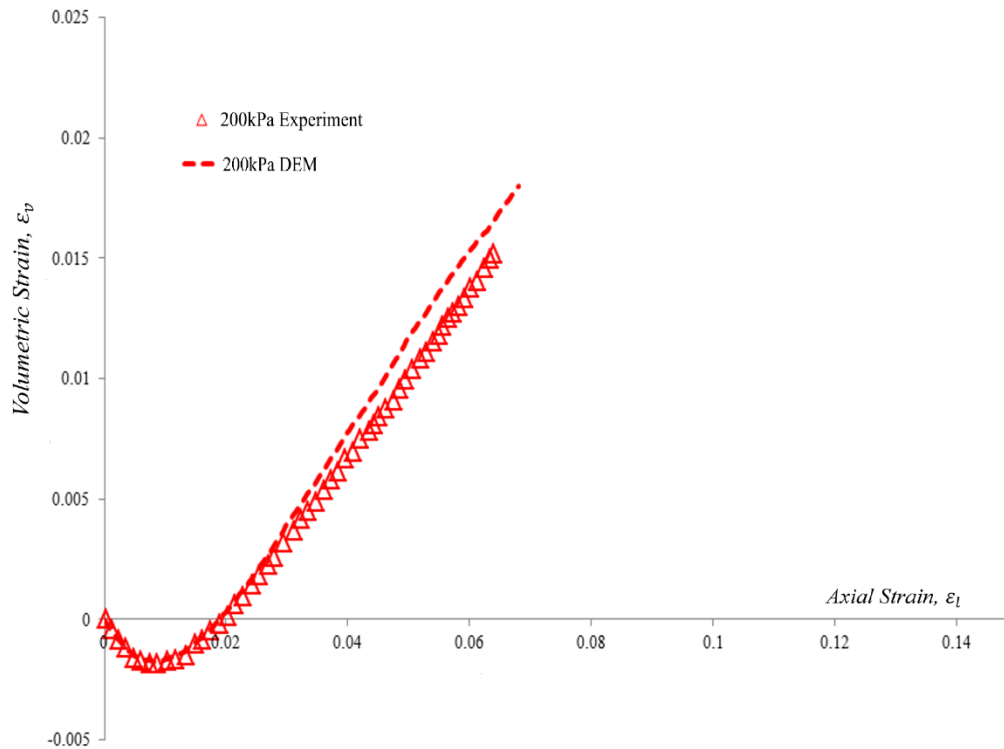


Figure 4.2.2.10 Dry specimen under triaxial compression, plotted with the experimental result, volumetric strain vs. axial strain, confining stress=200 kPa.

4.2.3 Discussion

Microscopic parameters including the coefficient of rolling resistance, angle of interparticle friction and normal and tangential stiffness were firstly studied to better understand their macroscopic effects. As a calibration method, numerical dry triaxial tests were conducted to simulate laboratory tests of Labenne sand which had a similar grading curve to LB sand fraction E. It was found that the DEM model is able to reproduce some of the major characteristics and mechanical properties of the laboratory triaxial tests. In terms of the deformation curve, a good agreement was obtained between the numerical model and practical granular material. However, a difference was found between the gradient of the stress-strain curves. The difference could result from the relatively small quantity of particles in an assembly (about 8,000), or the small

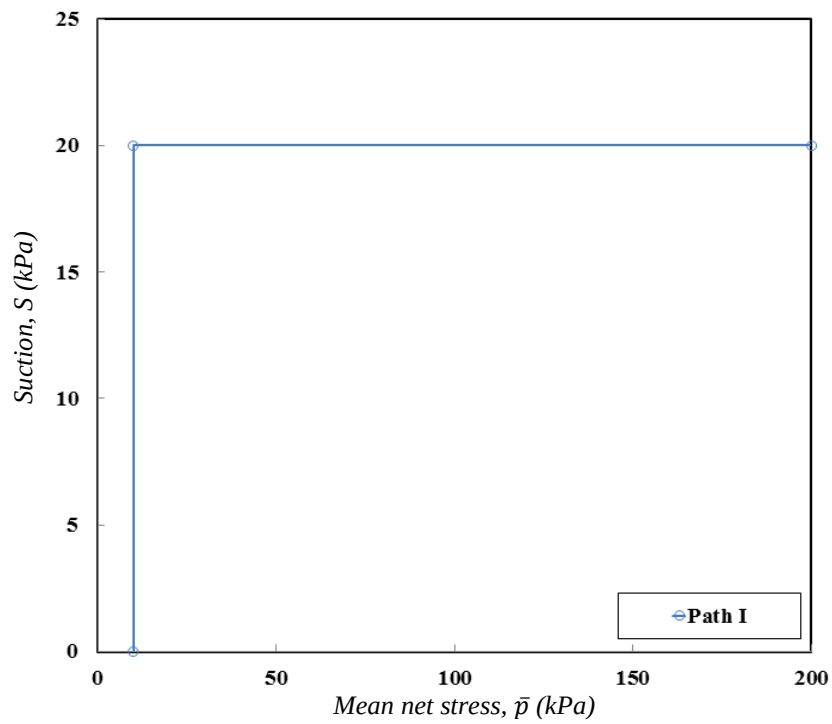
assembly size (50mm cube). The rolling resistance was introduced since the spherical particles in LIGGGHTS lacked any representation of surface roughness. It was found that the peak stress was highly dependent on the rolling resistance, however it had little influence on the deformation curve. It was also noted that normal contact stiffness k_n , and the ratio of shear to normal contact stiffness $\frac{k_s}{k_n}$ dominated the deformation characteristics. k_n was also found to be influential on the initial gradient of the stress-strain relation curve. Furthermore, it was noticed that the dilatancy was also dependent on the Young's modulus and the interparticle friction.

4.3 Mechanical Behaviour of Unsaturated Soils

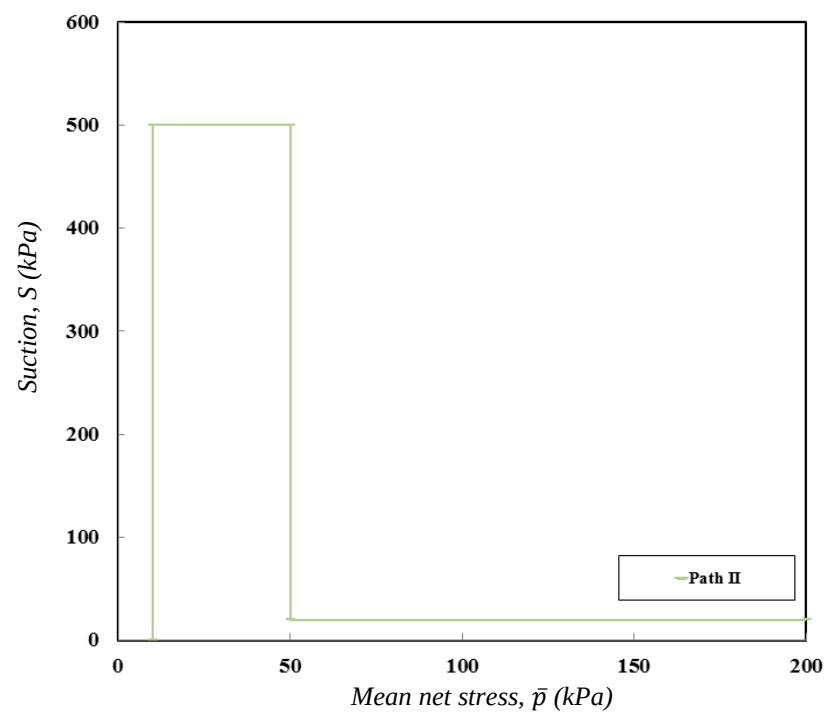
4.3.1 Preliminary Study with Unsaturated Materials

4.3.1.1 Isotropic compression with different wetting paths

Two different loading paths were also investigated in this study. For loading path I, a suction of 20kPa was imposed on the numerical assembly when the mean net stress reached 10kPa. For loading path II, a simple wetting process was simulated by imposing a suction of 500kPa when the mean net stress achieved 10kPa, reducing to 10kPa when the stress reached 50kPa. Figure 4.3.1.1 plotted the loading paths I and II. In Figure 4.3.1.2, the evolution of void ratio and saturation degree under the isotropic compression for both loading paths is plotted against the mean net stress.



(a) path I, suction=0-20kPa



(b) path II, suction=500kPa-0kPa

Figure 4.3.1.1 Loading paths for suction controlled isotropic compression.

It can be found in Figure 4.3.1.2 that a relatively smaller void ratio was produced when loading path II was adopted. However, the same value of void ratio was produced when the confining stress reached 200kPa. A small reduction in the mean net stress could also be found in loading path II when a higher water content was imposed ($S = 20kPa$). Figure 4.3.1.3 shows that an identical saturation degree was generated for both loading paths. No major difference could be found using different wetting paths during the isotropic compression for the numerical assembly. In this study, isotropic compression was firstly applied to the dry assemblies, and the capillary bridge model was only implemented before the triaxial test.

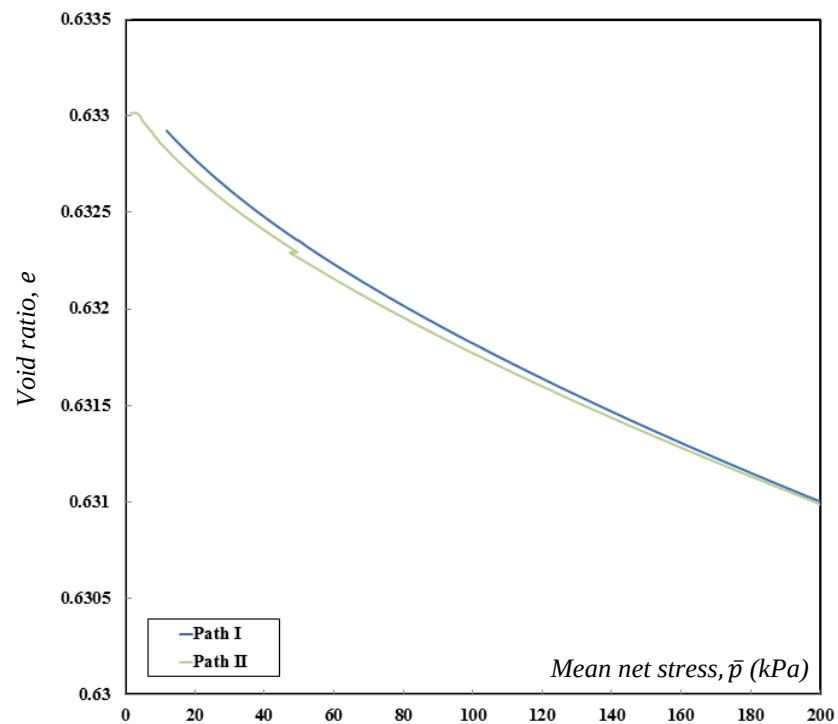


Figure 4.3.1.2 Suction controlled isotropic compressions under different loading paths, void ratio vs. mean net stress.

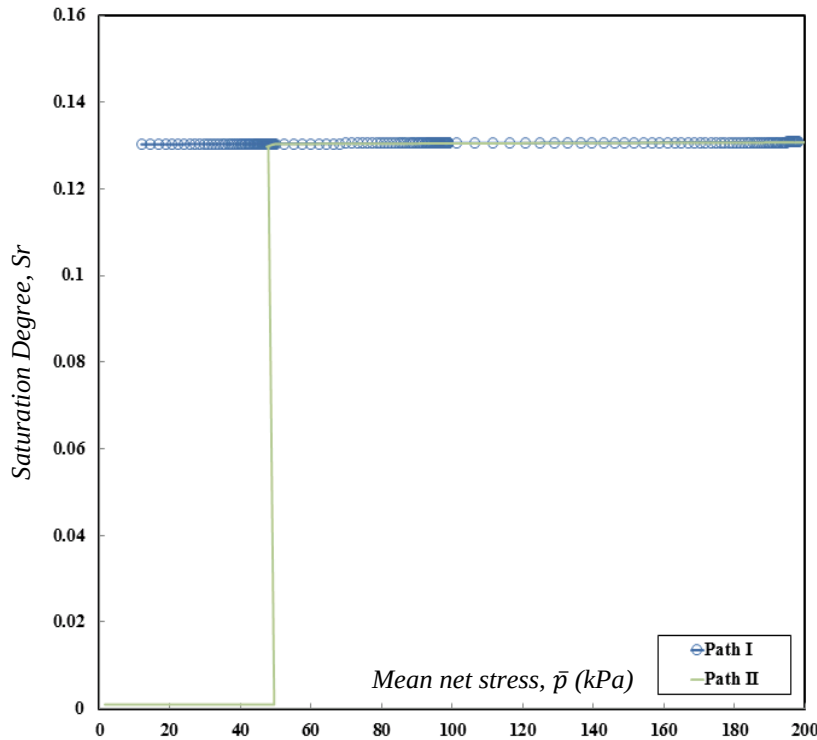


Figure 4.3.1.3 Suction controlled isotropic compressions under different loading paths, saturation degree vs. mean net stress.

4.3.1.2 Soil water characteristic curve

It could be concluded from previous studies that the mechanical behaviour of unsaturated soil could be significantly influenced by its hydraulic properties. For a constant value of matric suction, the volume of each capillary bridge formed in a particle assembly could be estimated by applying the toroidal approximation method. The saturation degree of the assembly then could be determined by calculating the total volumes of void spaces and capillary bridges. Using the toroidal approximation method, soil water characteristic curves (SWCCs) of the particle assemblies with different void ratios were produced to further investigate the hydraulic properties produced in numerical simulations. Using a temperature pressure cell and capillary rise open tube, the drying and wetting SWCCs for five sandy soils were investigated by Yang *et al.* (2004). To avoid

the effect of particle size on matric suction, all values of suction were converted into the dimensionless form ($S^* = \frac{2R_m S}{T}$). The degrees of saturation were also limited within the range of the pendular regime, which was assumed as 16% in this study. Using the same model for estimating the capillary bridge, the numerical SWCCs were then plotted by Wang (2014) in Figure 4.3.1.3, comparing with the experimental SWCCs for gravelly sand ($D_m = 4.7mm$) and fine sand ($D_m = 4.7mm$).

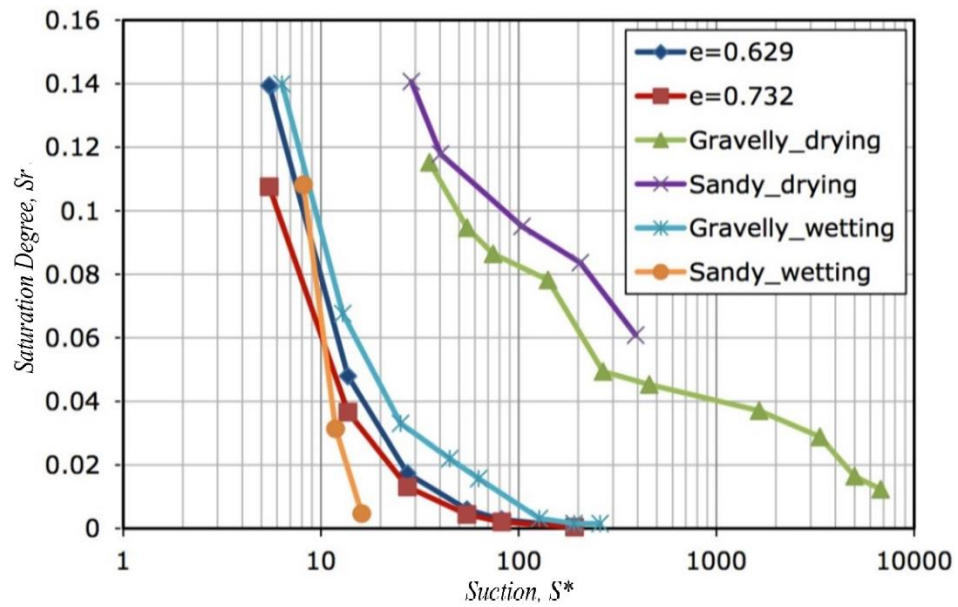


Figure 4.3.1.4 SWCCs for numerical samples and experimental results (Wang, 2014).

It could be found that the soil water retention properties of the unsaturated granular assemblies, with capillary bridges produced by the toroidal approximation method were close to the experimental results of wetting paths of fine sand and gravelly sand. It indicated the validity of the toroidal approximation in the hydraulic property, especially in modelling the wetting paths for fine sand and gravelly sand. However, much higher saturation degrees could be found from the drying paths of experimental results. Since the contact angle was configured to be 0° in the numerical model to achieve the highest

water content, the simulation results of SWCCs also showed the underestimation of water content when applying this method. For an unsaturated soil assembly, this could lead to a less significant strengthening effect on the macroscopic stress-strain behaviour.

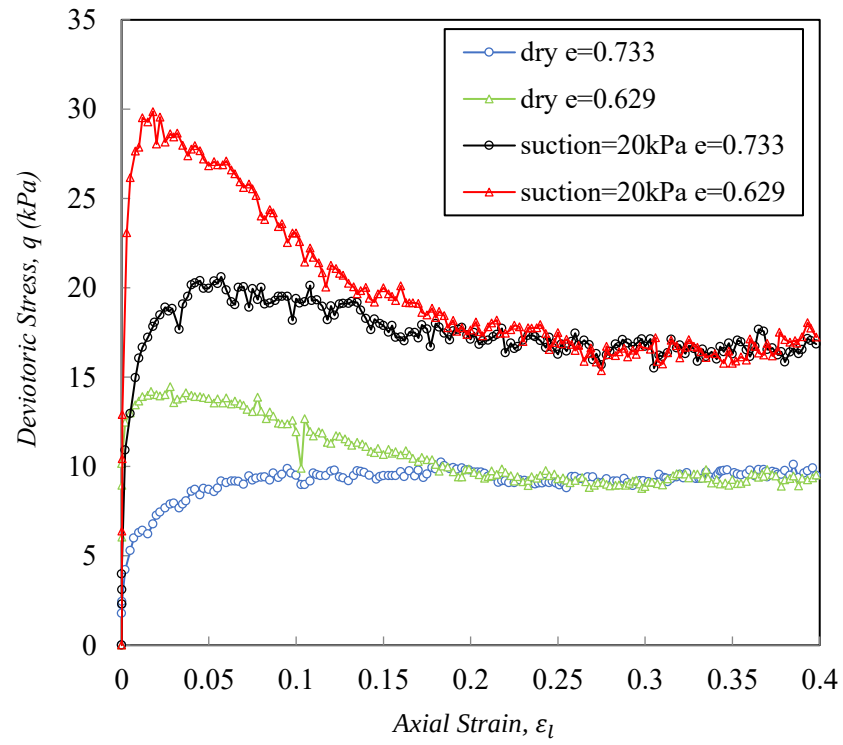
4.3.2 Triaxial Test Simulations

4.3.2.1 Triaxial shearing to critical state

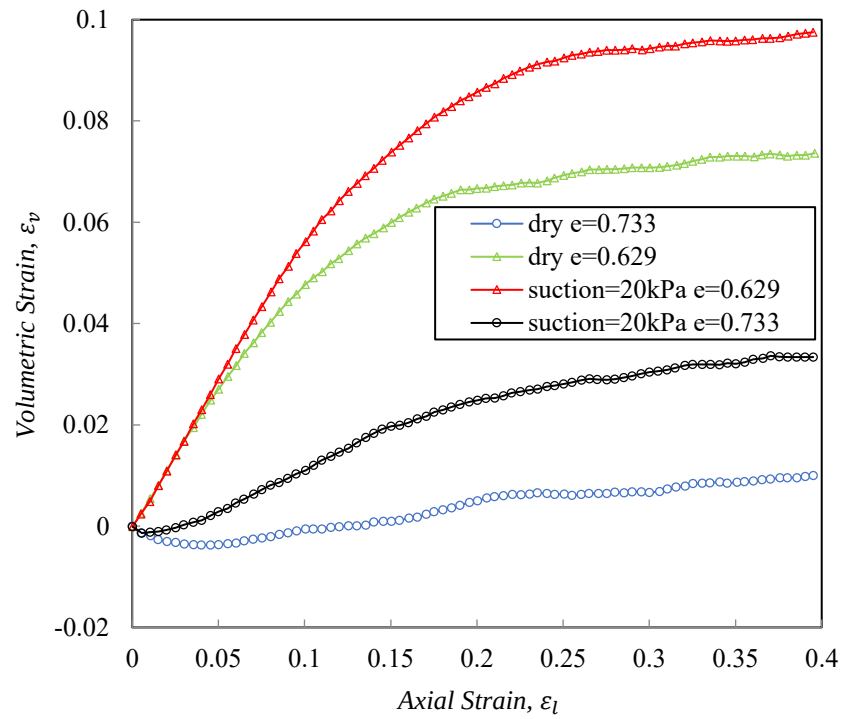
The critical state of the soil in this study refers to the specific behaviour of a soil assembly in triaxial shearing. At the beginning of the critical state, shear deformation could occur without any further changes in deviatoric stress, mean effective stress, void ratio and specific volume.

To investigate the critical state of unsaturated materials, triaxial test simulations were carried out using two numerical assemblies with different void ratios ($e = 0.733$ and 0.629) and the same confining stress ($\sigma_2 = \sigma_3 = 10kPa$). Uniform distribution of capillary effect was adopted. The mechanical behaviour for both dry and unsaturated conditions ($S = 20kPa$) is presented in Figure 4.3.2.1.

The evolution of the deviatoric stress, volumetric strain, void ratio and saturation degree of both assemblies is plotted against axial strain. It could be found that constant values were achieved by all variables while the axial strains generally reached 0.4.



(a) deviatoric stress vs. axial strain

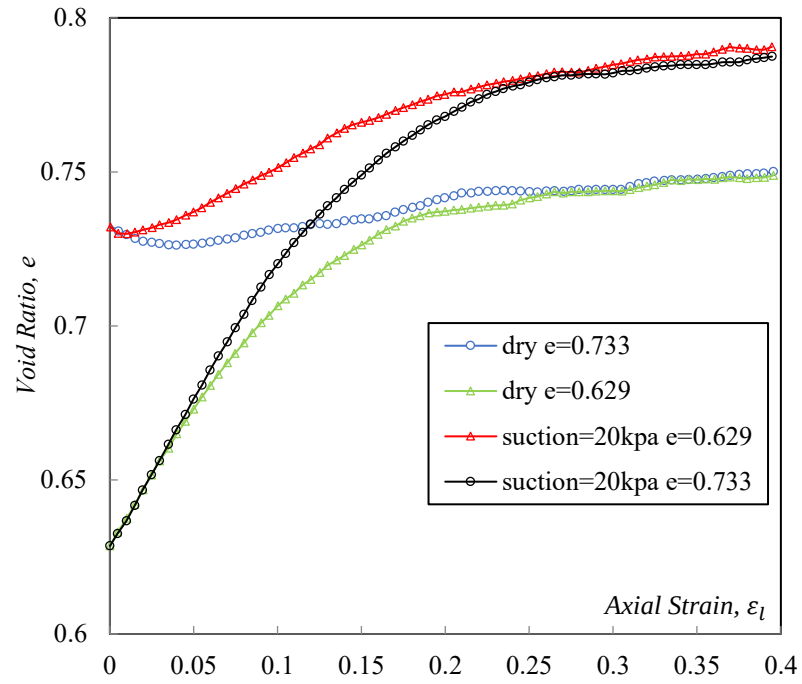


(b) volumetric strain vs. axial strain.

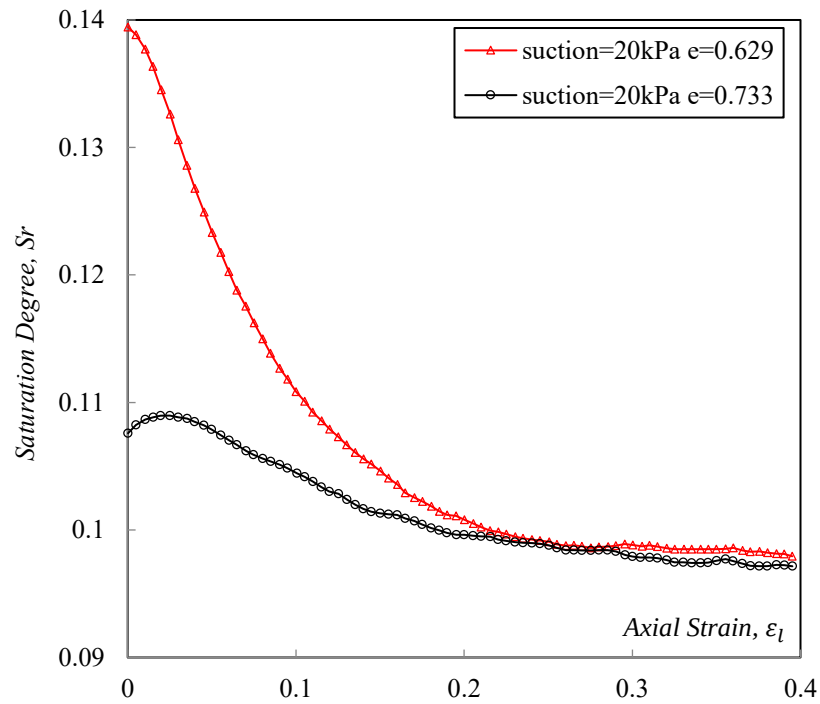
Figure 4.3.2.1 Dry and unsaturated granular materials ($S = 20\text{kPa}$) sheared to the critical state ($\sigma_2 = \sigma_3 = 10\text{kPa}$), (i).

It could be found in Figure 4.3.2.1a that the shear strength of the materials was significantly improved by the capillary effect. For materials with the same void ratio, the ultimate deviatoric stresses were found as equivalent despite the difference in their initial states. Figure 4.3.2.1b presents the deformation behaviour of both numerical assemblies with different void ratios. It could be determined that capillary effects significantly raised the dilatancy, leading to much higher ultimate volumetric strains in unsaturated materials.

The evolution of void ratio during triaxial shearing is illustrated in Figure 4.3.2.2a. The values of void ratio in all specimens generally increased until reaching the critical state. Moreover, nearly identical values of void ratios could be found to be *c.* 0.788 for the unsaturated assemblies and *c.* 0.728 for dry specimens. A larger void ratio was found in unsaturated materials, which could result from multiple reasons. Firstly, the appearance of the water phase could be an important factor. Due to the water surface tension and the cohesive force developed from the capillary bridge, a larger pore space could be tolerated by an unsaturated granular material. An identical saturation degree was achieved by both unsaturated assemblies with different densities, although their initial saturation degrees varied (Figure 4.3.2.2b). This could possibly result from identical void ratios at the critical state. As suction remained constant during the triaxial test simulation, the decreasing saturation degree and the increasing void ratio moreover could imply a reduction in capillary bridge number. Investigation into the microscopic parameters of unsaturated materials was conducted and will be presented in a later chapter.



(a) void ratio vs. axial strain



(b) saturation degree vs. axial strain.

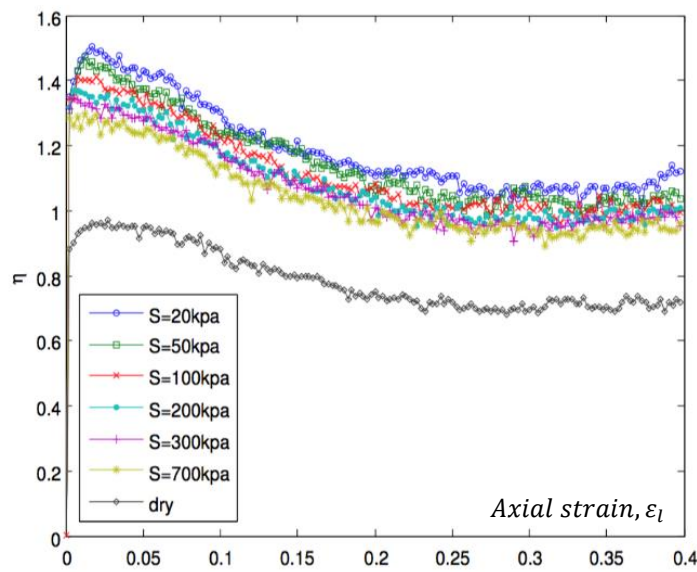
Figure 4.3.2.2 Dry and unsaturated granular materials ($S = 20\text{kPa}$) sheared to the critical state ($\sigma_2 = \sigma_3 = 10\text{kPa}$), (ii).

4.3.2.2 Influence of capillary cohesion

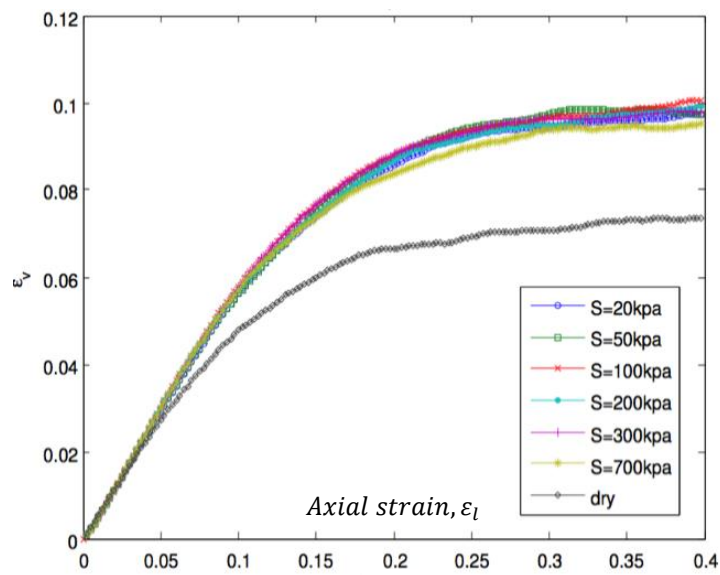
A series of numerical triaxial tests were carried out by Wang (2014) using a numerical assembly with a void ratio of 0.629. As the previous study, the same capillary bridge model with uniform water distribution was adopted. Different values of matric suction were applied to the assembly, which had a confining pressure of 10kPa and a mean particle radius of 0.01mm. Figure 4.3.2.3 shows the evolution of stress ratio (η) and volumetric strain (ϵ_v) of the unsaturated assembly under triaxial shearing. The stress ratio is defined as the ratio of the deviatoric stress to the mean normal stress. It could be found that the stress ratio was significantly increased due to the appearance of capillary cohesion, and that higher stress ratio could be achieved when lower suctions were applied. Compared to the dry material, an increase in the volumetric strain also could be found in unsaturated assembly. These results show that the formation of capillary bridges had a strengthening effect on the granular material. They may suggest that, in pendular states, the toroidal approximation of capillary bridges could be an efficient method for investigating the macroscopic behaviour of unsaturated materials that is influenced by the capillary effect.

As a preliminary study of the stress-strain behaviour of unsaturated granular materials, numerical triaxial tests were also carried out with numerical assemblies under different confining pressures ($\sigma_2 = \sigma_3 = 50\text{kPa}$ and 200kPa). The value of matric suction was configured as 20kPa for all unsaturated materials. Assemblies with different void ratios ($e = 0.629, 0.68$ and 0.733) were also produced to investigate the influence of packing efficiency. By comparing Figure 4.3.2.3a and Figure 4.3.2.3b, it could be found that the effect

of capillary cohesion decreased when a higher confining stress was applied. One of the reasons for the unapparent capillary effect under high confining stress could be the relatively large particle size. Although a similar void ratio was achieved compared to real soil materials, much smaller particles with wider size distribution were involved in practical problems. Some attributes of the capillary bridge model could also be the important factors, for example, the estimated external and internal radii of the menisci.

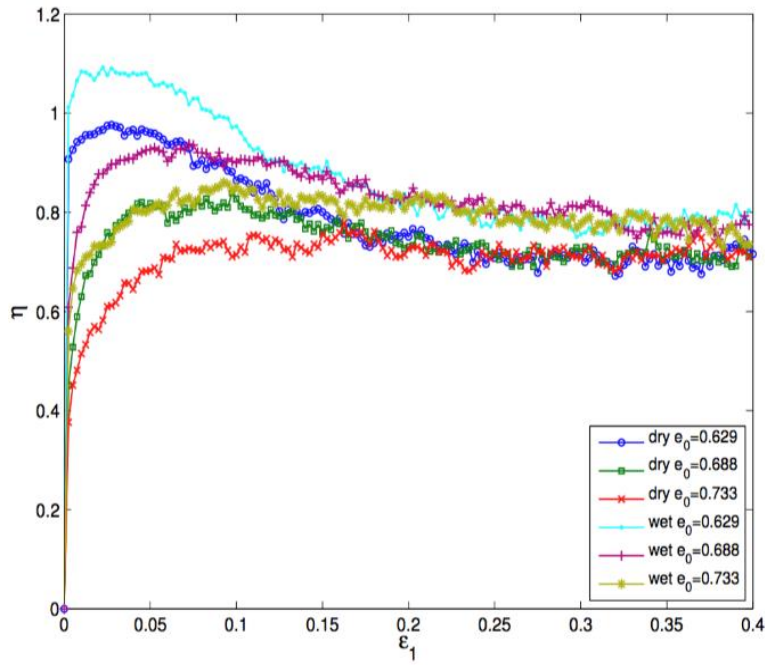


(a) stress ratio vs. axial strain

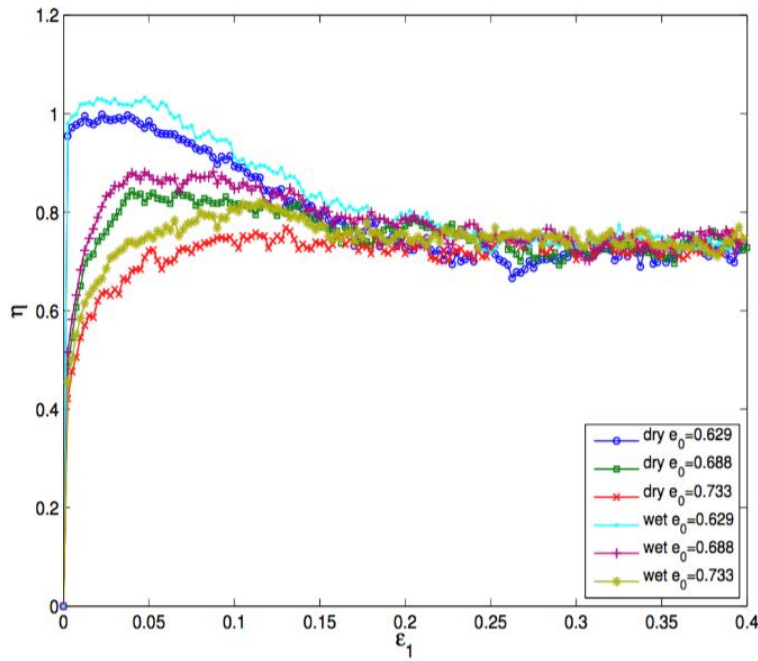


(b) volumetric strain vs. axial strain

Figure 4.3.2.3 Triaxial tests of unsaturated materials with uniform water distribution (Wang, 2014).



(a) $\sigma_2 = \sigma_3 = 50 \text{ kPa}$



(b) $\sigma_2 = \sigma_3 = 200 \text{ kPa}$

Figure 4.3.2.4 Evolution of deviatoric stress with different confining stresses (Wang, 2014).

4.3.3 Discussion

In the preliminary study of unsaturated material, the soil water characteristic curves (SWCCs) were firstly generated for the numerical samples using the toroidal approximation method. It could be noticed that higher saturation degree was generated when lower suction value was applied. The SWCCs of the unsaturated specimens were found to be close to the experimental results of the wetting paths of fine sand and gravelly sand. The results of SWCCs also showed an underestimation of water content of the toroidal approximation method. For unsaturated soil materials in pendular states, this could lead to a decreased strengthening effect on the macroscopic stress-strain behaviour.

The stress-strain behaviour of unsaturated materials were presented with a series of suction values. It was found that higher stress ratio could be achieved when applying lower suction value, *e.g.* higher saturation degree (Figure 4.3.2.1a). For an unsaturated material in the pendular state, results may indicate that higher saturation degree could lead to the increased number of capillary bridges, and eventually result in a larger value of stress ratio. As the liquid phase was assumed as uniformly distributed, and only capillary bridges would be generated when two particles were within the rupture distance, the increased material strength could result from the increased number of capillary bridges which could eventually develop cohesive forces between solid particles. In practical problems, however, the liquid phase is more likely to be randomly distributed in an unsaturated granular material. A smaller number of capillary bridges might be generated in an unsaturated material when the liquid phase is only partially distributed. Results also showed a decreased strengthening effect when higher

confining stress was involved. According to previous studies, the particle size could be a significant factor influencing the magnitude of capillary effect. It was found that higher strengthening effect could be generated when smaller particle size was adopted.

4.4 Liquid Distribution in Wet Granular Materials

4.4.1 Distribution Models for Capillary Bridge

To investigate the influence of the spatial distribution of capillary bridges by numerical modelling, different distribution models for capillary bridges were introduced and investigated in this study. It was assumed that capillary bridges could form in certain volume percentage of a particle assembly. Two different particle types (x and y) were used in simulations, and capillary bridges were only allowed to form between type y particles. Different distribution models were established by dividing the cubic assembly into different regions, and configuring specific particle types in specific regions.

Figure 4.4.1.1 demonstrates the numerical assemblies with capillary bridges distributed in different specific regions in the yz plane. The blue areas represent the regions with capillary bridge formation, and all granules in white areas were assumed as dry particles. From models $I_{25\%}$ to $VI_{25\%}$, 25% of the entire volume of each assembly was permissible for the formation of capillary bridges (Figure 4.4.1.1a), while 75% of the entire volume was used from models $I_{75\%}$ to $V_{75\%}$ (Figure 4.4.1.1b). The percentage value was defined as the liquid volume fraction in this study.

The 3D illustration of model II_{75%} is also demonstrated in Figure 4.4.1.1b, where the blue particles represent the ones that were allowed for capillary bridge formation. A void ratio of 0.633 and a constant suction of 20kPa were imposed to all distribution models.

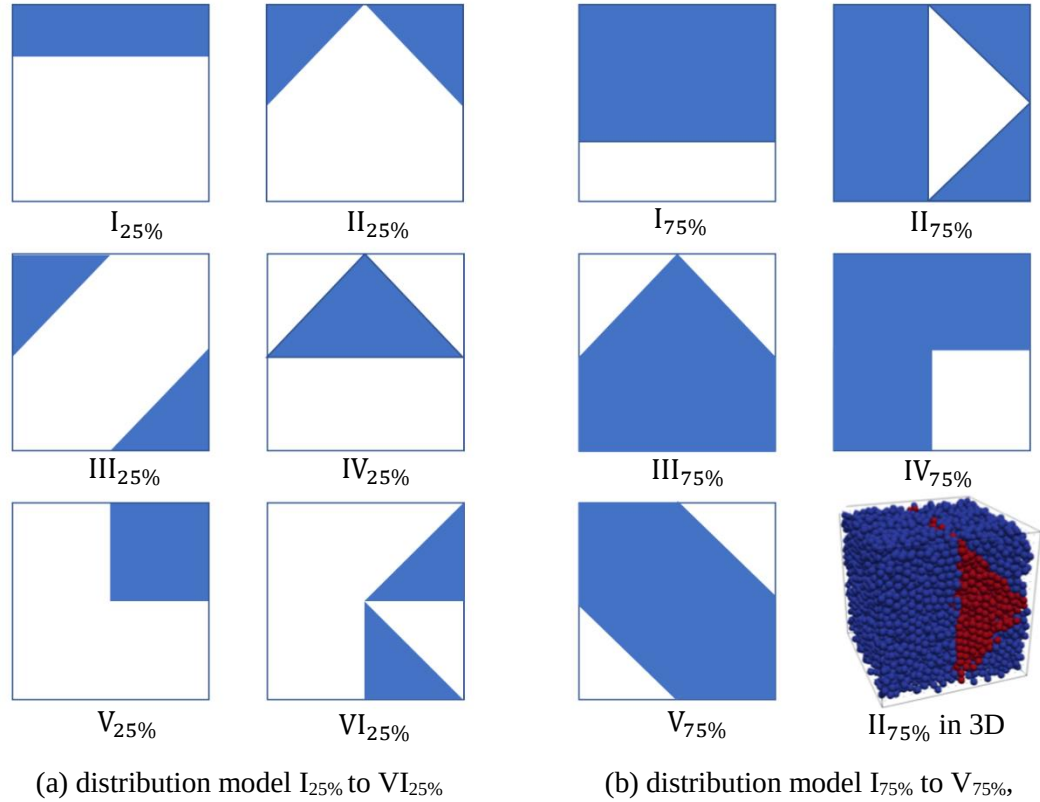


Figure 4.4.1.1 Water distribution models with 25% and 75% liquid volume fraction.

4.4.2 Influence of Liquid Distribution

4.4.2.1 Soil Water Characteristic Curves

Using the toroidal approximation method, soil water characteristic curves (SWCC) were produced specifically for every distribution model. Figure 4.4.2.1 illustrates the SWCCs for models I_{25%} to V_{25%}. Similar results were found from these models. For assemblies with low values of total suction, higher water

volumes could be found from model $IV_{25\%}$ and $V_{25\%}$. In contrast, Model $II_{25\%}$ had the lowest water content when applying same values of suction.

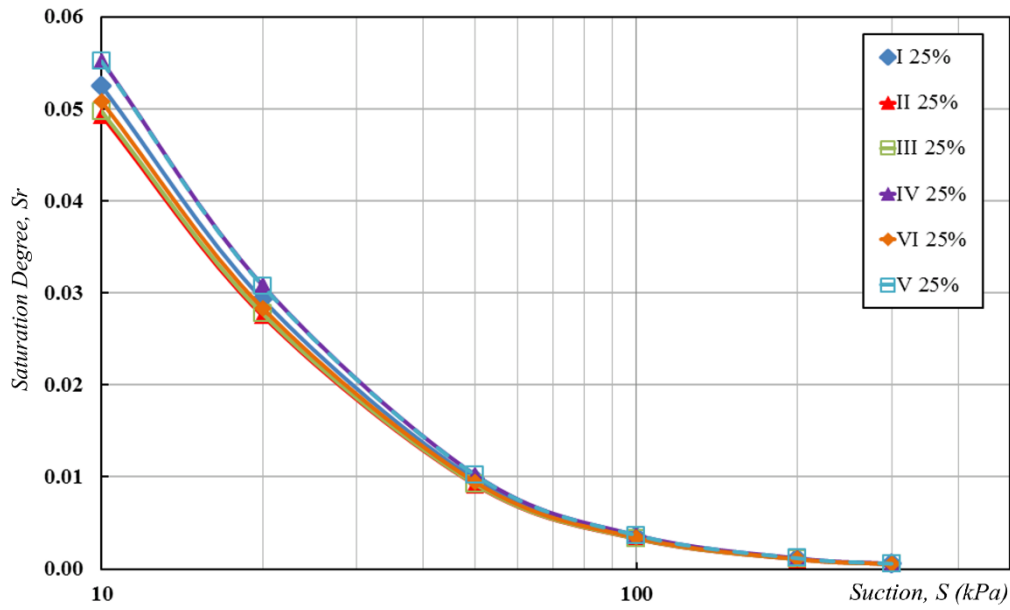


Figure 4.4.2.1 SWCCs plotted for water distribution models $I_{25\%}$ to $VI_{25\%}$.

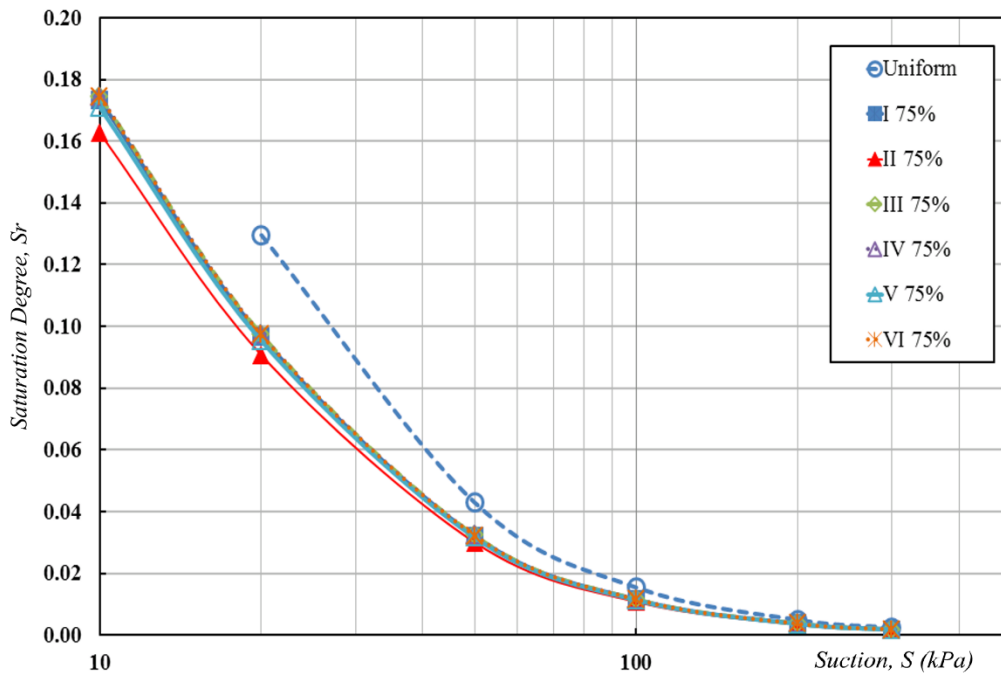


Figure 4.4.2.2 SWCCs plotted for water distribution models $I_{75\%}$ to $V_{75\%}$.

Figure 4.4.2.2 plots the SWCCs for models $I_{75\%}$ to $V_{75\%}$. The SWCC with uniform distribution of capillary bridge is also plotted on the same graph for

comparison. It could be found that model II_{75%} had the lowest water content when the same suctions were applied. Besides that, identical SWCCs were produced by models I_{75%} to V_{75%}. The similarity of these SWCCs justifies the uniform distribution of pore space in the particle assembly after isotropic compression.

By comparing Figure 4.4.2.1 and Figure 4.2.2.2, it could be observed that higher saturation degree was achieved by models with larger liquid volume fraction. The maximum value of water content appeared to occur when water was uniformly distributed in the numerical assembly (Figure 4.2.2.2). To investigate the influence of liquid distribution on the mechanical behaviour of unsaturated granular materials, triaxial test simulations were carried out for these models with different liquid distributions.

4.4.2.2 Triaxial Shearing of different distribution models

To investigate the influence of liquid distribution on the mechanical behaviour of wet granular materials, triaxial test simulations were carried out for different distribution models. Constant values of suction ($S = 20\text{kPa}$), void ratio ($e = 0.63$) and confining stress ($\sigma_1 = \sigma_2 = 10\text{kPa}$) were adopted in all the simulations to observe the influence of different water distribution patterns. As shown in Figure 4.4.2.1 and Figure 4.4.2.2 higher saturation degree could be achieved for water distribution models with larger liquid volume fraction. Figure 4.4.2.3a shows the stress ratio against axial strain for models I_{25%} to VI_{25%}, and Figure 4.4.2.3b presents the deformation behaviour of these models. The same curves are plotted for models I_{75%} to V_{75%} in Figure 4.4.2.5.

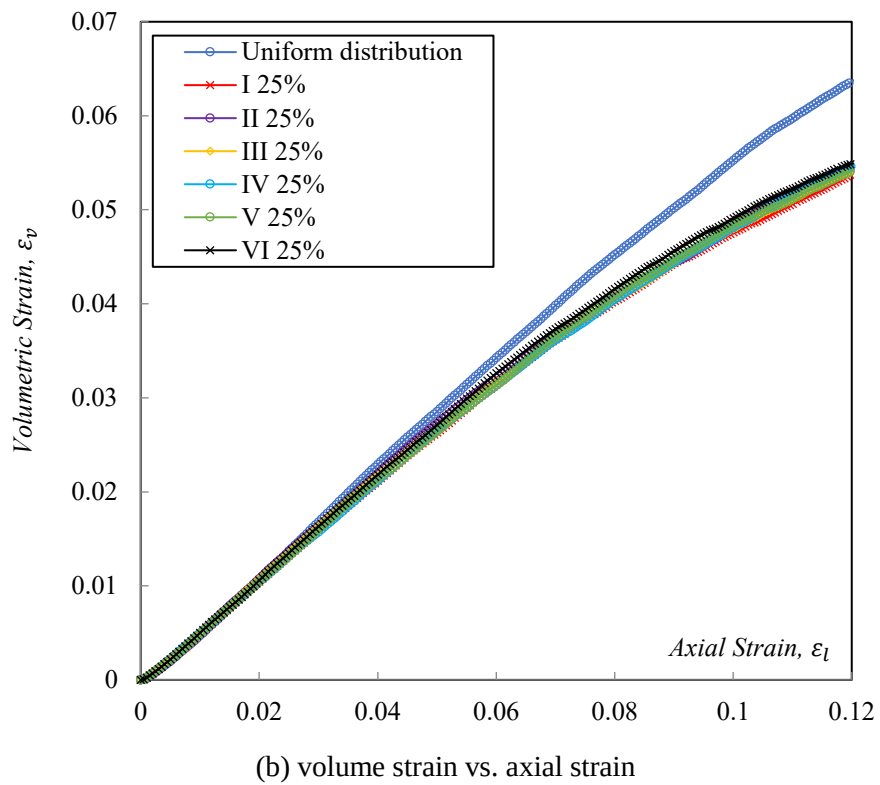
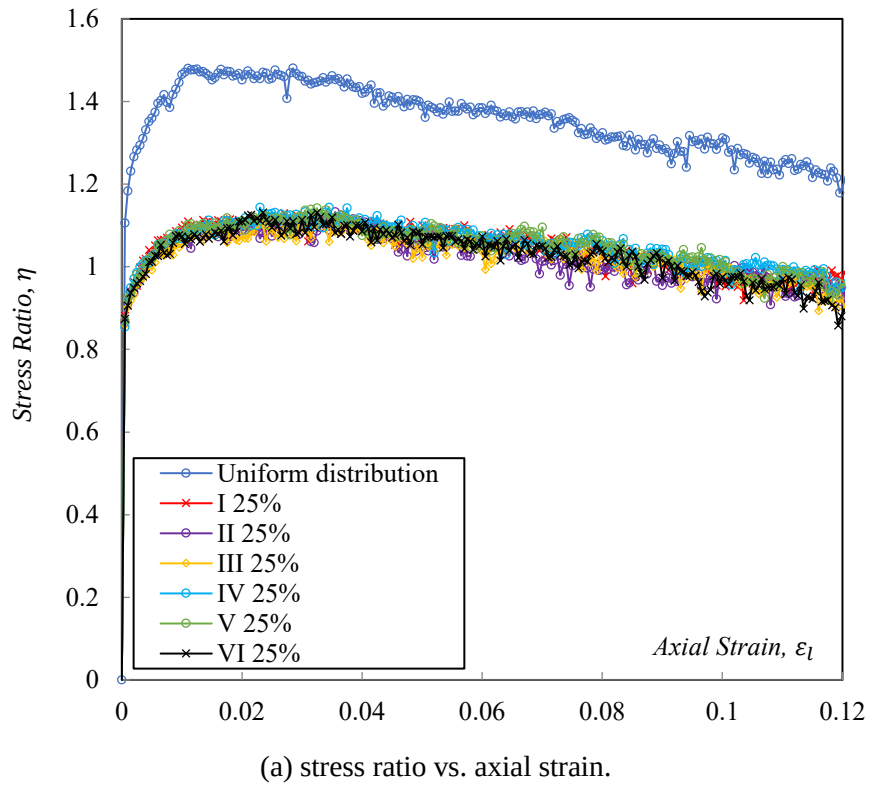
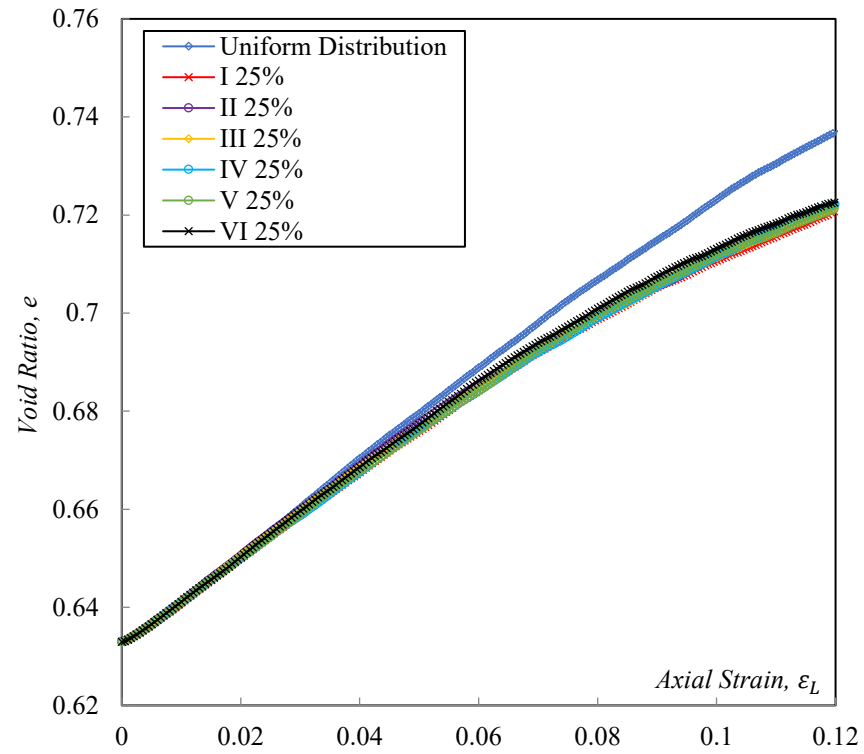
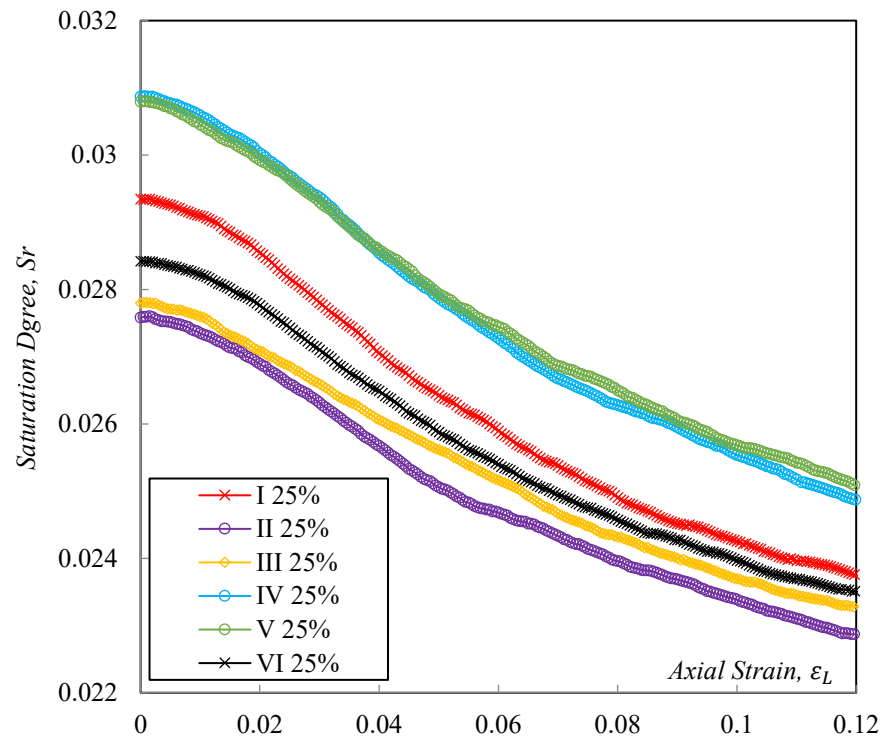


Figure 4.4.2.3 Triaxial tests simulations for models $I_{25\%}$ - $VI_{25\%}$, ($S = 20 \text{ kPa}$), (i).

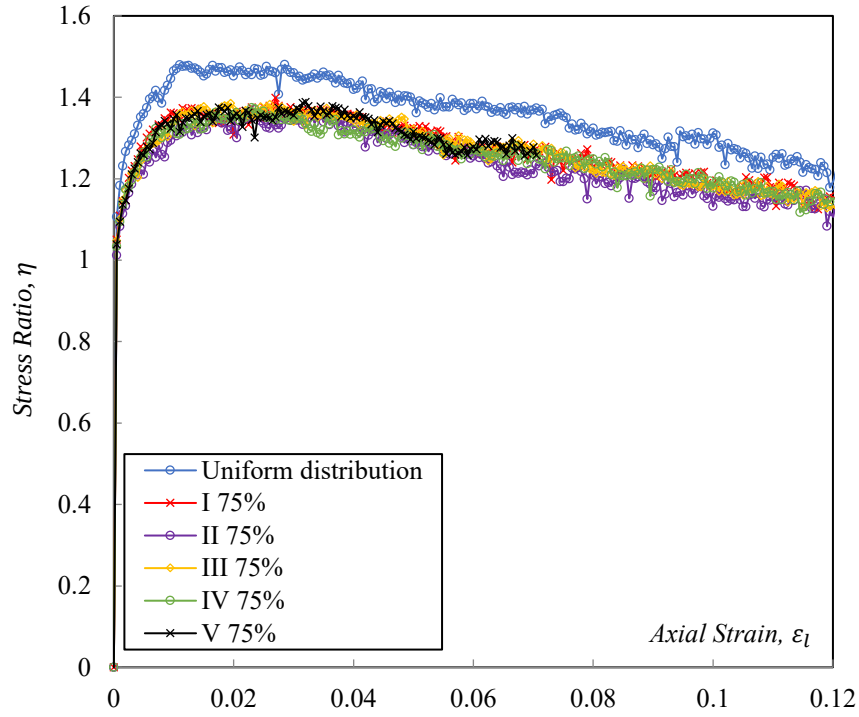


(a) void ratio vs. axial strain

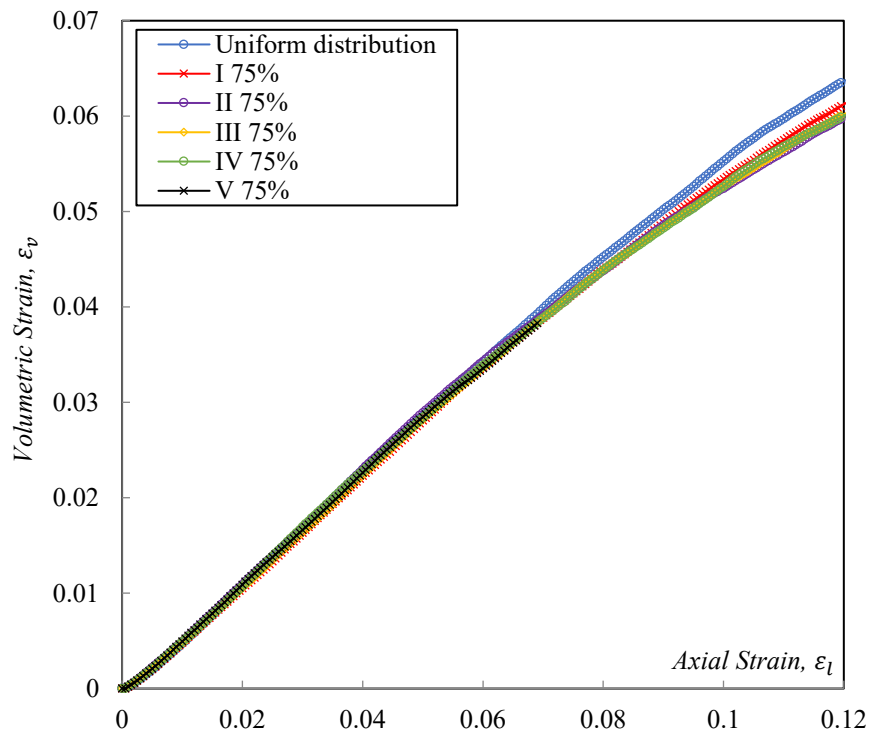


(b) saturation degree vs. axial strain

Figure 4.4.2.4 Triaxial tests simulations for models $I_{25\%}$ - $VI_{25\%}$, ($S = 20 \text{ kPa}$), (ii).

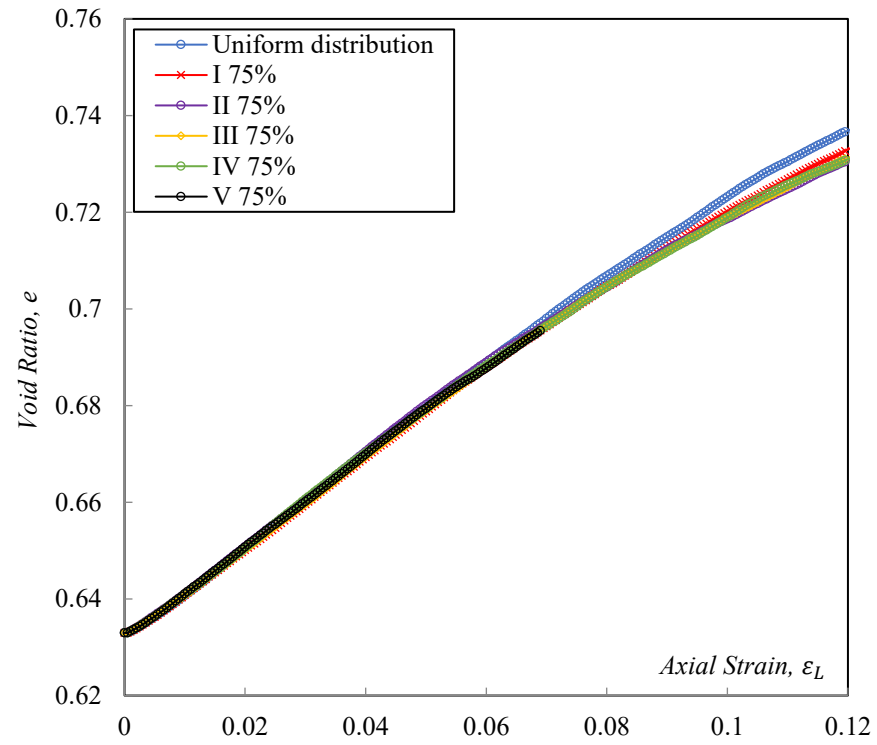


(a) stress ratio vs. axial strain.

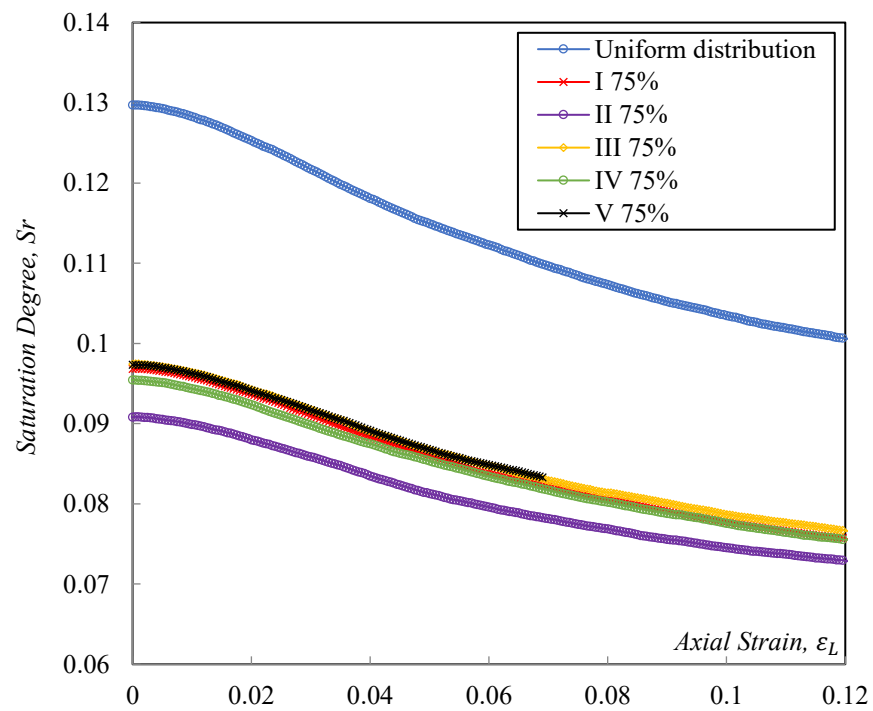


(b) volume strain vs. axial strain

Figure 4.4.2.5 Triaxial tests simulations for models $I_{75\%}$ - $V_{75\%}$, ($S = 20 \text{ kPa}$), (i).



(a) void ratio vs. axial strain



(b) saturation degree vs. axial strain

Figure 4.4.2.6 Triaxial tests simulations for models I_{75%}-V_{75%}, ($S = 20 \text{ kPa}$), (ii).

For assemblies with the same volume percent for capillary bridge formation, similar stress-strain behaviour could be found in Figure 4.4.2.3 and Figure 4.4.2.5 respectively. It may imply that the distribution of the water phase only had limited influence on the macroscopic behaviour of an unsaturated material.

By comparing Figure 4.4.2.3a and Figure 4.4.2.5a, it could be found that a higher stress ratio could be achieved by models with higher volume percent for capillary bridge formation. The higher material strengths could be concluded as the results of higher water contents. Compared to the unsaturated assembly with a uniform water distribution, it was found that the volume range for capillary bridge formation could be another important factor leading to the variation of the material strength. Moreover, no significant change in the dilatancy could be found between models with different liquid volumes. This reveals that the range of water distribution does not affect the deformation of an unsaturated assembly.

It could be concluded that the distribution of liquid phase had little influence on the macroscopic stress-strain behaviour. In the pendular regime, a higher water content leads to a higher strength of an unsaturated assembly. Nevertheless, it is important not to neglect the influence from the spatial range of capillary bridges. Because of the similarity in the macroscopic behaviour, simplified distribution models were applied for further investigations.

4.4.3 Distribution models with the same degrees of saturation

4.4.3.1 Simplified distribution models

Since similar macroscopic behaviour could be found from different distribution models, simplified distribution models could be applied for further investigations. To study and understand their mechanical behaviour, the simplified liquid distribution models $I_{25\%}$ and $I_{75\%}$ were presented where capillary effects were assigned to 25% and 75% of the volumes were assigned capillary effects (Figure 4.4.3.1). The results from the previous section revealed the significance of the water distribution magnitude, and the saturation degree might not be the only factor affecting the material strength. Suction controlled triaxial test simulations was later conducted with the simplified models to further investigate the influence of water distribution in unsaturated materials.

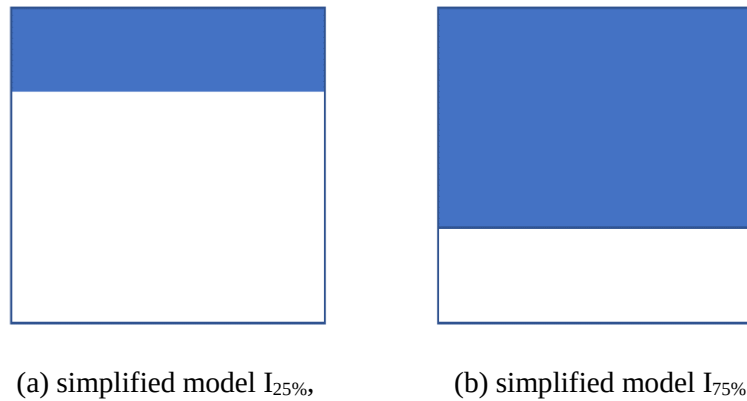


Figure 4.4.3.1 Simplified models for liquid distribution.

4.4.3.2 Influence of liquid distribution on macroscopic behaviour

Firstly, the total saturation degree was configured to be c. 4% for both specimens by imposing suctions according to the SWCC curves produced earlier (Figure 4.4.2.1 and Figure 4.4.2.2). Triaxial test simulations were carried out for both specimens with different magnitudes of capillary effects.

The evolutions of the macroscopic parameters, including stress ratio, volumetric strain and saturation degree were plotted in Figure 4.4.3.2 and Figure 4.4.3.3.

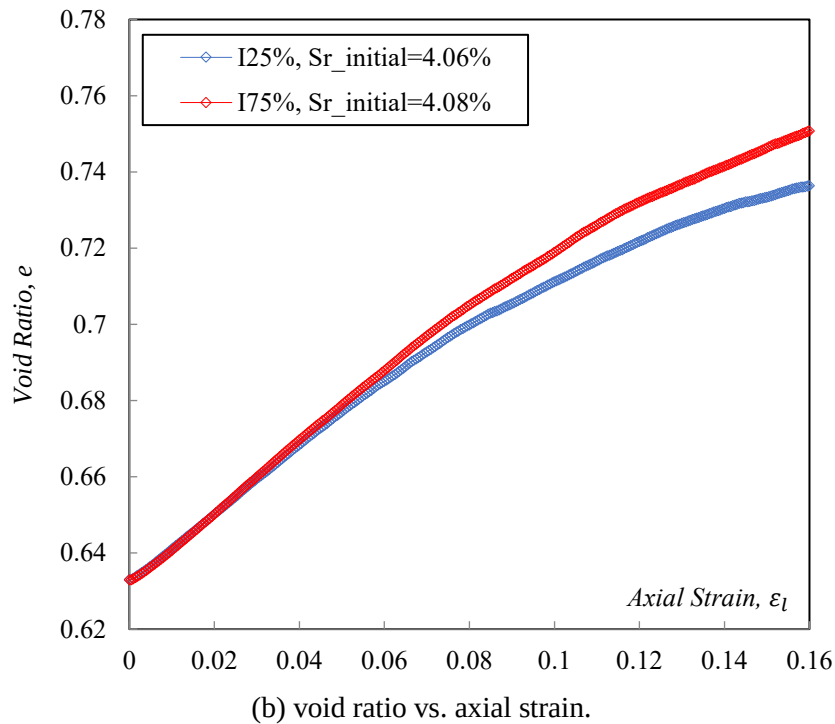
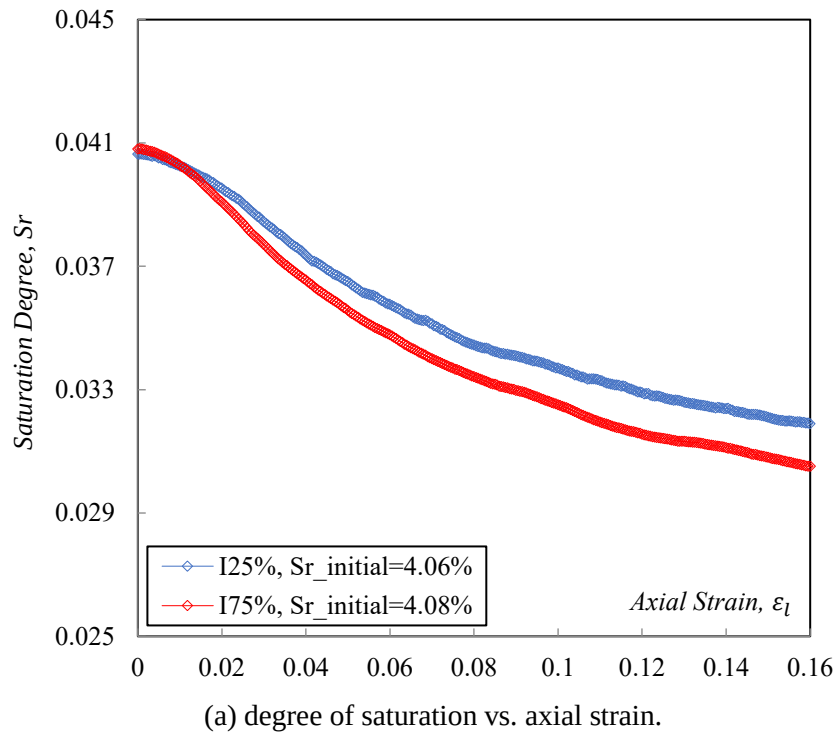


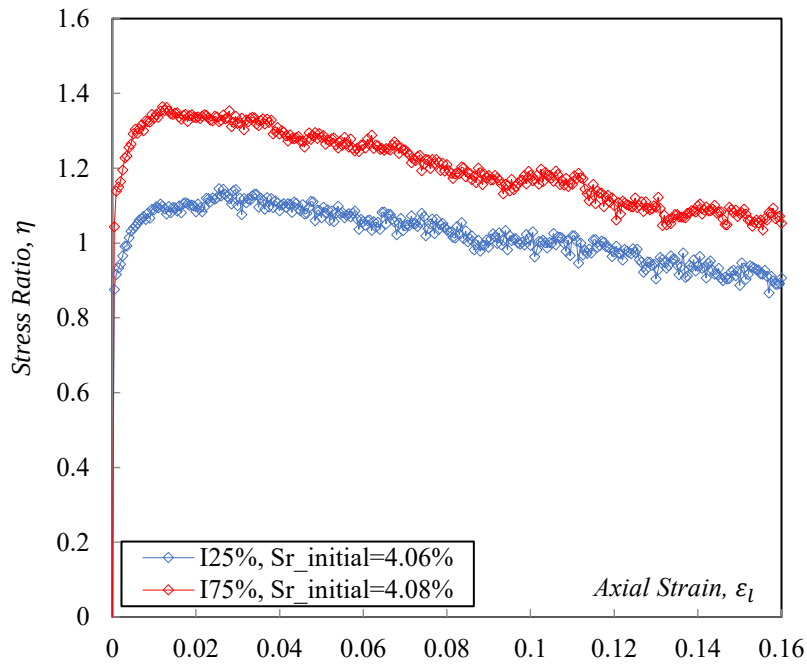
Figure 4.4.3.2 Triaxial test simulations for models I_{25%} and I_{75%} with identical saturation degrees, (i).

Firstly, Figure 4.4.3.2a shows the evolution of degree of saturation of the simplified distribution models. It could be found that the initial degrees of saturation were approximately equivalent. A saturation degree of 4.06% was achieved in model I_{25%}, and a value of 4.08% was produced in model I_{75%}. While the axial strain increased during the triaxial compression, a higher decreasing rate of the saturation degree could be observed from the specimen with larger liquid volume fraction (I_{75%}). It indicates that a smaller water content was generated in sample I_{75%} comparing to I_{25%} during the triaxial compressions.

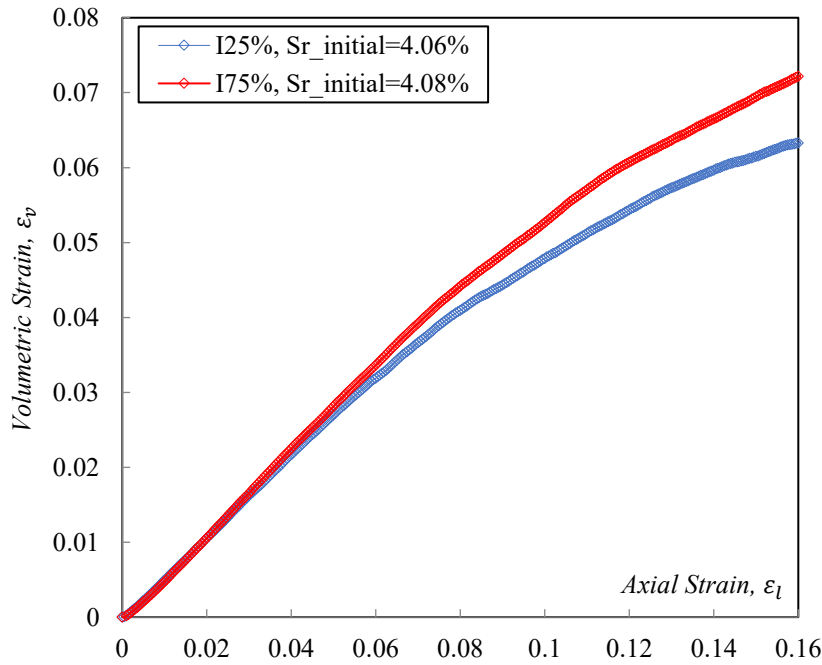
Figure 4.4.3.2b presents the developments of void ratio for both simplified models. Identical void ratio could be observed before the triaxial compression. It could be found that larger void ratio was generated in model I_{75%} after the triaxial compression took place. This could result from the smaller amount of water in model I_{75%} due to the lack of capillary cohesion. Since larger saturation degree was produced in model I_{25%}, smaller pore spaces might also result from the capillary effects.

Furthermore, Figure 4.4.3.3a plots the stress ratios against axial strains for both models under the triaxial stress path. A much higher stress ratio could be found from model I_{75%} compared to model I_{25%}. It was interesting to note that, larger stress ratio could be achieved by model I_{75%} although larger void space and smaller saturation degree was generated. These results could indicate the significance of the spatial distribution of water phase in an unsaturated granular material. It could be concluded that for an unsaturated material in the pendular state, a wider spatial range of capillary effects might lead to a higher strength.

The volumetric strain of both specimens was also plotted in Figure 4.4.3b, where larger volumetric strain also appeared to be achieved by model $I_{75\%}$.



(a) volume strain vs. axial strain



(b) void ratio vs. axial strain

Figure 4.4.3.3 Triaxial test simulations for models $I_{25\%}$ and $I_{75\%}$ with identical saturation degrees, (ii).

4.4.3.3 Effect of particle size

To investigate the effect of particle size in unsaturated material, numerical assemblies were generated using spherical particles with radii of 0.1mm to compare with the specimens adopted previously ($r = 0.01\text{mm}$). A void ratio of 0.633 and a constant suction of 20kPa were imposed for all specimens. The capillary effect was adopted using both the uniform distribution and the simplified distribution models $I_{25\%}$ and $I_{75\%}$. The mechanical behaviour of the numerical specimens under triaxial compression was plotted in the figures below. Figure 4.4.3.4a presents the evolution of stress ratio for each unsaturated specimen. It could be found that significantly larger stress ratios were produced in the specimens with smaller radii. For numerical assemblies consisting of larger particles, only a minor difference could be found in the stress ratio when different liquid volume fractions were involved. This indicates the significance of particle size in the development of capillary straining effect. Stronger capillary effect was generated when smaller particles were adopted.

The development of the volumetric strain was presented for each numerical specimen in Figure 4.4.3.4b. For unsaturated specimens with smaller particle size, the smallest volumetric strain could be determined in model $I_{25\%}$ while the largest value was generated by the model with uniform water distribution. However, only minor difference in volumetric strain could be found in the specimens with larger particles. This is because the volume change is highly dependent on the produced stress ratio. It could be found in Figure 4.4.3.4a that the stress ratios produced by specimens with larger particles were close to the

value generated in model I_{25%} with smaller particles. This could explain the similarity of their volumetric strains.

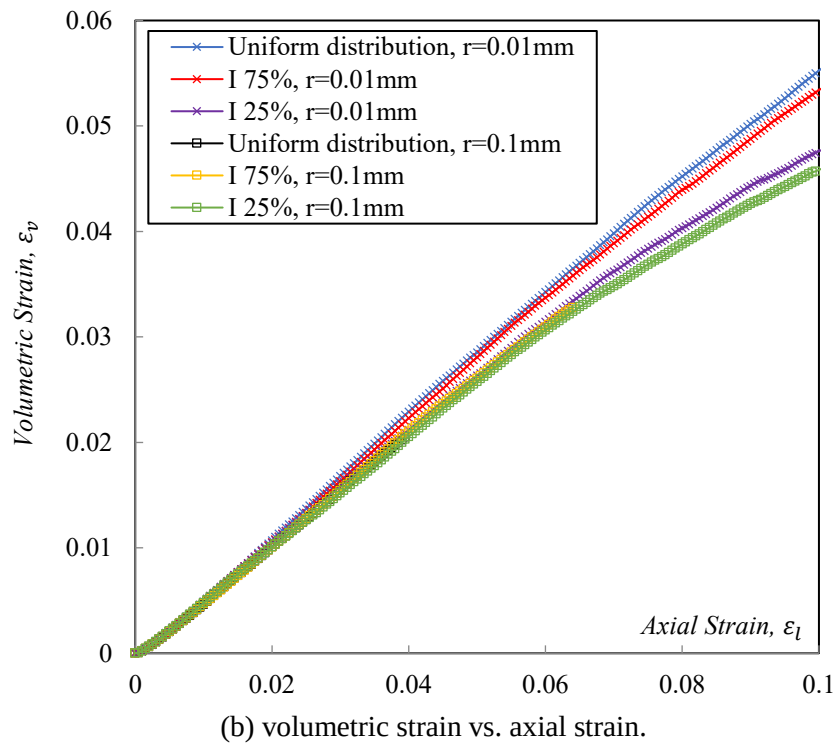
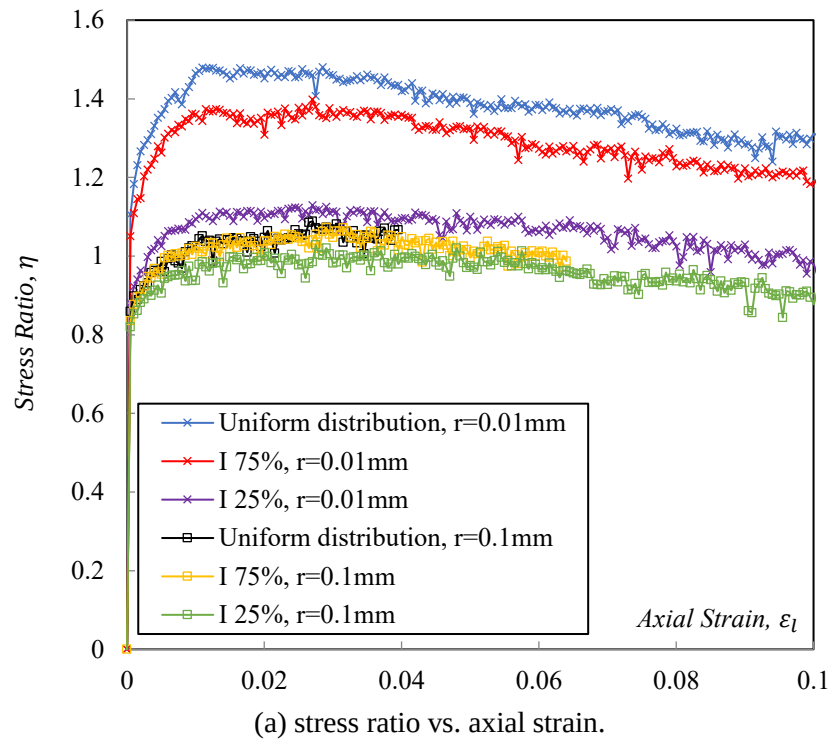


Figure 4.4.3.4 Triaxial test simulations for specimens with different particle size and varied water distribution.

Figure 4.4.3.5 presents the evolution of void ratio against axial strain for all unsaturated specimens. The largest void ratio was achieved by the numerical specimen with uniform water distribution and small particles ($r = 0.01\text{mm}$). Relatively larger differences in void ratios could be observed among the three unsaturated specimens with smaller particles. For specimens with the same particle size, moreover smaller void ratio could be detected when smaller liquid volume fraction was adopted. However, only a minor difference could be observed among the unsaturated specimens with larger particle ($r = 0.1\text{mm}$). Due to the void ratio evolution of an unsaturated granular material could be highly dependent on the volumetric strain, almost identical development could be found between the void ratio and the volumetric strain (Figure 4.4.3.5 and Figure 4.4.3.4b)

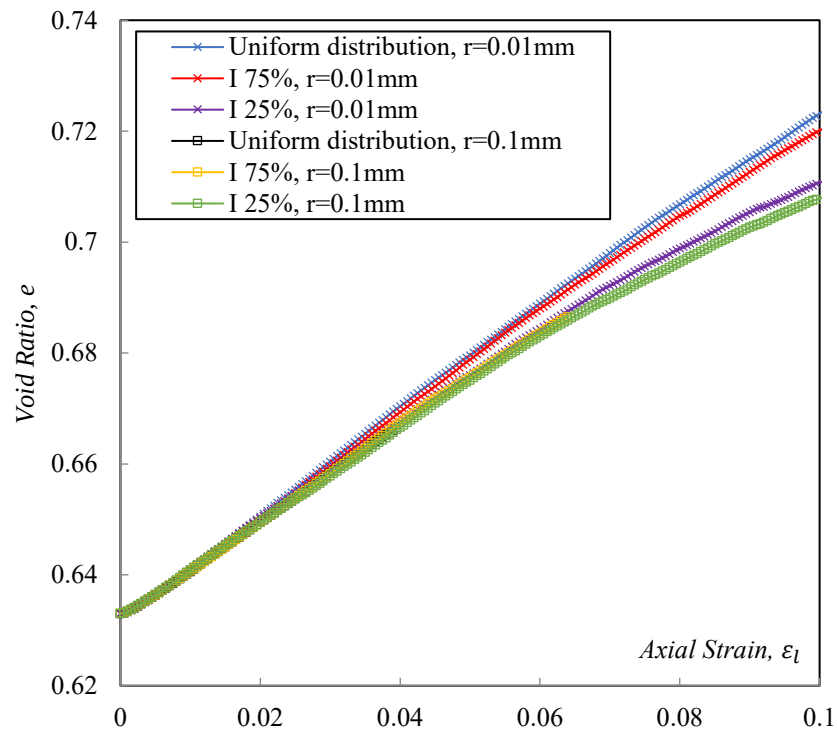


Figure 4.4.3.5 Triaxial test simulations for specimens with different particle size and varied water distribution, void ratio vs. axial strain.

Furthermore, the change of saturation degree in each specimen is also plotted in Figure 4.4.3.6. Identical values of saturation degree could be found in the specimens with the same liquid volume fraction. As smaller void ratio could be detected in the specimens with larger particle, the identical saturation degree could imply that the lower water content was generated. To further understand the influence of particle size on the capillary strengthening effect, microscopic investigations were carried out and are presented in chapter 6.

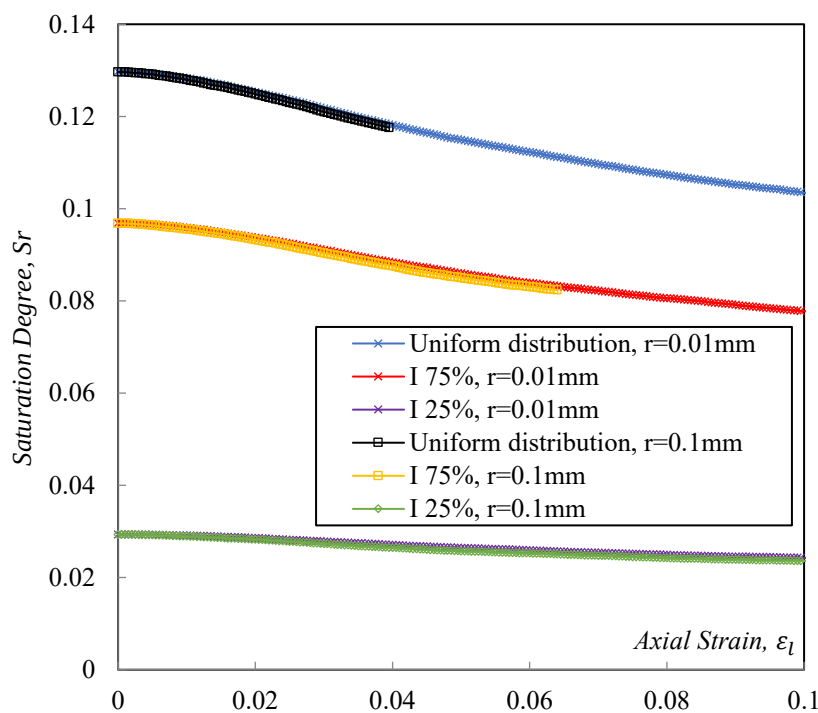


Figure 4.4.3.6 Triaxial test simulations for specimens with different particle size and varied water distribution, saturation degree vs. axial strain.

4.4.4 Discussion

A series of water distribution models for capillary bridges were presented to study the influence of liquid distribution in unsaturated materials. Various distribution models were presented specifically for numerical specimens with different liquid volume fractions (25% and 75%) where capillary bridge formation was permitted.

The SWCCs for all the water distribution models were firstly produced using the iterative method by imposing a constant local suction. The value of suction was configured to be 20kPa for every formed capillary bridge. In Figure 4.4.2.1 and Figure 4.4.2.2, similar results could be observed for the models with the same magnitude of liquid volume fraction. The similarity of these SWCCs indicated a uniform distribution of pore spaces in the particle assembly after the isotropic compression. Since only spherical particles with the same size was adopted, the uniform distribution of the pore structure can be achieved after an isotropic compression. Due to the constant suction was adopted in this study, the distance between a pair of particles thus becomes an important factor dominating the geometry of the capillary bridge which connects the particles. These may finally lead to the near-identical values of saturation degree.

By conducting the triaxial test simulations, higher stress ratios and larger dilatancy appeared to be achieved by unsaturated specimens with larger liquid volume fraction. Almost identical stress-strain behaviour could be found from all distribution models with the same magnitude of liquid volume fraction. Similar developments of stress ratios and volumetric strains could be found in Figure 4.4.2.3 and Figure 4.4.2.5. These observations may suggest that simplified water distribution models ($I_{25\%}$ and $I_{75\%}$) could be considered as good representatives for particle assemblies with the random water distribution but a certain liquid volume fraction.

By carrying out the triaxial test simulations using the simplified models ($I_{25\%}$ and $I_{75\%}$) with near-identical saturation degrees, higher stress ratio appeared to

be produced by the model with larger liquid volume fraction. This might imply that better strength and larger deformation could be generated when the same amount of liquid phase was more widely distributed in an unsaturated material. Thus, the liquid volume fraction could be another important factor dominating the strength of an unsaturated material. Since only capillary bridge can occur in simulations, more bridges can be developed when the same amount of water is more widely distributed. Therefore, the increased strength may result from the larger values of both water coordination number and solid coordination number, and the higher interparticle forces. Moreover, the stress ratio and the volumetric strain achieved by the model $I_{25\%}$ may be even lower in practice when compared to $I_{75\%}$, due to the water coordination number in DEM can be highly overestimated when the local saturation degree is relatively high.

Moreover, for numerical assemblies consisting of larger particles, only minor differences appeared in the stress ratio when different liquid volume fractions were involved. This could imply the importance of particle size in the development of capillary strengthening effect. A higher capillary strengthening effect appeared to be generated when smaller particles were adopted. These observations also show that relatively lower water content was generated in the specimens with larger particles, as larger void ratio could be detected. Future studies including the microscopic parameters are presented in chapter 6.

4.5 Summary

In this chapter, the strengthening effect of the capillary bridge was firstly confirmed in the suction controlled triaxial test simulations. For an unsaturated

granular material in the pendular regime, it was found that the increasing total water content could result in a higher shear strength. The results also showed that the capillary strengthening effect might also be increased with the density of particles. Moreover, it could also be concluded that the capillary effect significantly raises the dilatancy, leading to a much higher ultimate volumetric strain in the unsaturated material.

Six water distribution models were introduced and studied in this chapter to investigate the influence of capillary bridge distribution. Suction-controlled triaxial tests were conducted for all the distribution models, and macroscopic behaviour were investigated in this chapter. Observations appeared to show that the distribution of liquid phase had little influence on the macroscopic stress-strain behaviour. Higher stress ratios and volumetric strains could be developed by applying the larger liquid volume fraction (75%). These results might indicate that for unsaturated assemblies with the random water distribution and a certain liquid volume fraction, the simplified water distribution models ($I_{25\%}$ and $I_{75\%}$) could be good representatives.

By conducting the triaxial tests with the simplified models, a much higher stress ratio could be observed with the model $I_{75\%}$ when near-identical saturation degrees were adopted. These results appeared to indicate that for an unsaturated material in the pendular state, a wider spatial range of capillary bridges could lead to a higher material strength. The stress-strain behaviour of an unsaturated material might be better predicted in practice when incorporating the estimation of the liquid volume fraction.

CHAPTER 5: Statistical Analysis with X-ray Computed Tomography

5.1 Introduction

The previous section confirmed that for most granular materials at low water content, such as unsaturated soils, their strengths could be increased by capillary cohesion developed at the particle-liquid contacts. In general DEM simulations, the analytical solution usually assumes that the magnitude of the capillary forces depends on the liquid surface tension and the radii of curvature of the capillary bridge. The contact angle of the air-liquid interface against the surface of the solid particles was considered as the only factor dominating the radii of curvature. Additionally, capillary bridges are usually assumed to be concave, generating tensile capillary pressure.

However, evidence from previous research has mainly come from theoretical studies or experimental observations at the millimetre scale (Lourenço *et al.*, 2011). To further understand the interplay between the mechanical properties and the water content, the geometric information and spatial distribution of capillary bridges were investigated using x-ray computed tomography (XRCT). In this study, tests were carried out using specimens filled with spherical glass beads ($r = 0.1\text{mm}$). A constant value of target porosity (0.43) was imposed on all three specimens with a series of target saturation degrees ($Sr_t = 6\%$, 9% and 12%). The total mass and the total volume of each unsaturated specimen were measured and controlled to achieve a similar porosity.

5.2 Three Phases of Unsaturated Material

5.2.1 Air Phase and Porosity

A variety of target saturation degrees were generated in three assemblies consisting of spherical glass beads to produce a set of idealised unsaturated specimens. By applying the iterative threshold to the image slices, the pore space firstly could be segmented to calculate the porosity of the specimens. Figure 5.2.1.1 presents both 2D and 3D views of specimen I, which had a target saturation degree of 6%. The highlighted blue area represents the pore space in the specimen, which includes the air phase and the liquid phase. The black areas in the 2D image were the removed particle phases. By deleting the particle phase, the porosity of the specimen therefore could be determined by calculating the volume fraction of the pore space over the total space under scan.

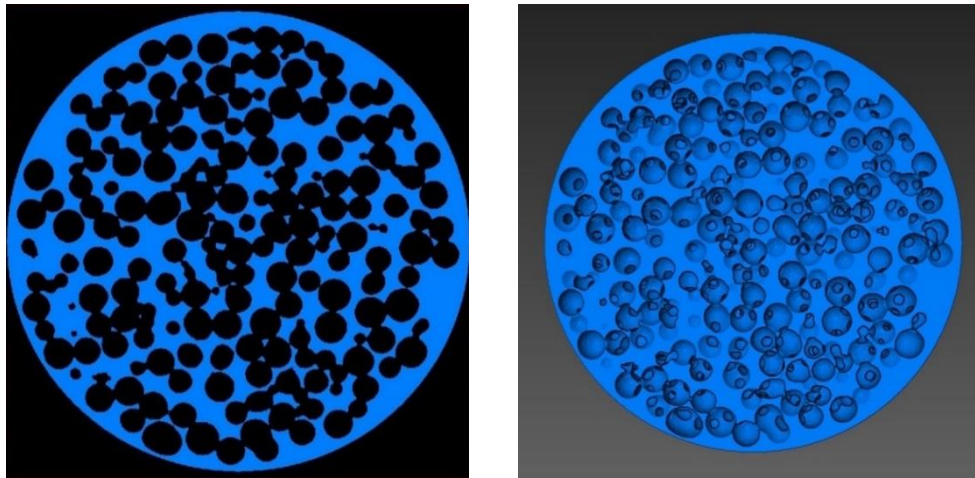


Figure 5.2.1.1 2D and 3D views of the pore space in specimen I (Target $S_r=6\%$).

Table 5.2.1.1 presents the porosity of each specimen calculated using this method. The porosity of the specimen was controlled to be 0.43 in this study, according to the published data of typical maximum porosities of gravelly sands and fine sands ([Geotechdata, 2013](#)). A relatively larger porosity of 0.45 could be found in specimen I which had the least amount of water. Near-identical porosity

values were generated in specimen II and III, which were 0.425 and 0.424 respectively.

Table 5.2.2.1 Estimated porosities by image analysis.

	Pore volume (μm)	Total volume (μm)	Porosity
Specimen I ($Sr_t=6\%$)	1.19E+11	2.62E+11	0.453
Specimen II ($Sr_t=9\%$)	1.11E+11	2.61E+11	0.425
Specimen III ($Sr_t=12\%$)	1.11E+11	2.62E+11	0.424

Similarly, the porosity in specimen II which had a target saturation degree of 9% was determined using the same approach. Figure 5.2.1.2 shows the pore space of the specimen in both 2D and 3D. Figure 5.2.1.3 shows the pore space in specimen III, with a target saturation degree of 12%.

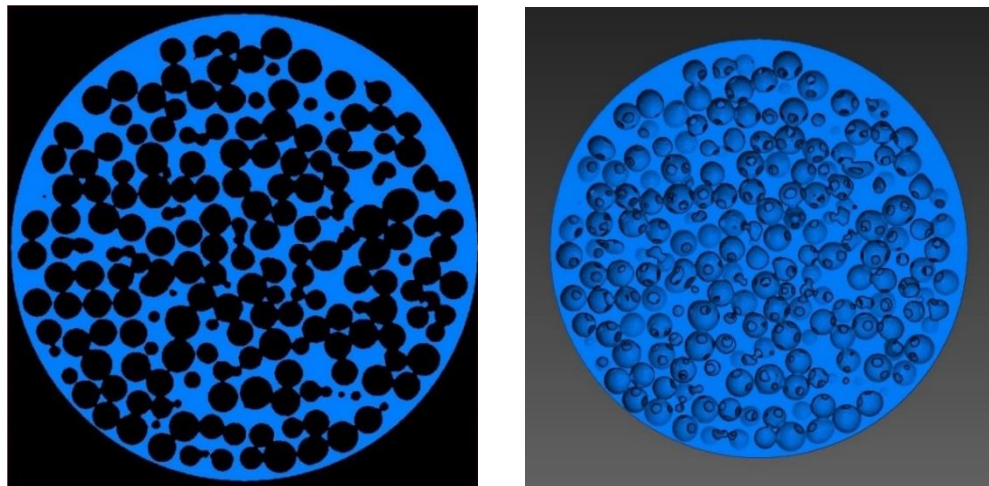


Figure 5.2.1.2 2D and 3D views of the pore space in specimen II (Target $Sr=9\%$).

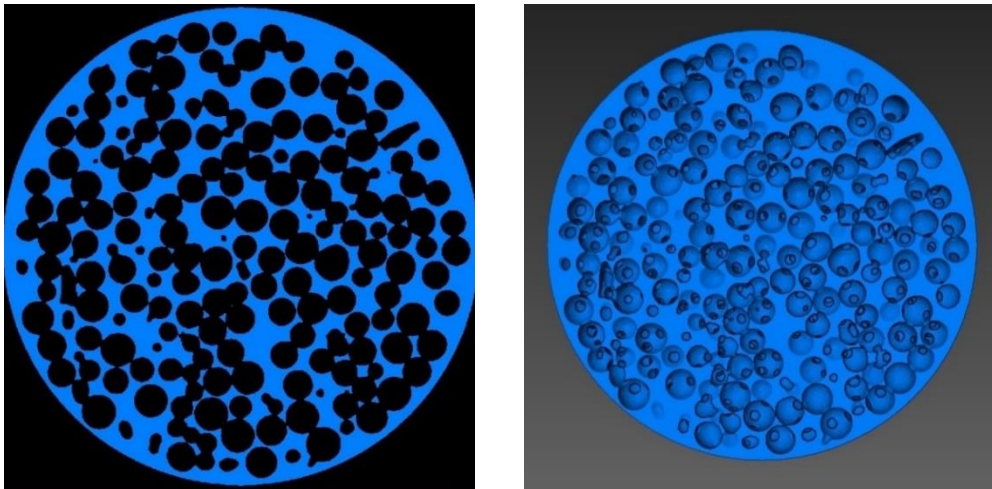


Figure 5.2.1.3 2D and 3D views of the pore space in specimen III (Target $S_r=12\%$).

By controlling the total mass and the total volume of the assembly of glass beads, similar values of porosities could be found among three specimens. The estimated porosities were found to be close to the target value of 0.43. Smaller porosity values were generated in specimens with higher saturation degree. This could result from the larger capillary cohesion generated by the increased saturation degree. During the procedure of isotropic compression, longer duration was required to achieve the same level of compression for specimens with less water content. Applying a series of isotropic compressions for unsaturated materials with different suction levels, similar phenomena also could be found in DEM simulations.

5.2.2 Liquid Phase and Saturation Degree

Specimens with a variety of target saturation degrees were produced to investigate the influence of capillary effects under low water content. By applying a specific range of iterative thresholds on the image slices, the liquid phase was segmented and highlighted in blue for sample specimen I which had

a saturation degree of 6% (Figure 5.2.2.1). Since the water was controlled to be uniformly distributed among the spherical glass beads, a small amount of liquid could be found to surround every particle. The 3D view shows that the surrounding water could help to form liquid films around particles, which finally could contribute to the development of capillary bridges.

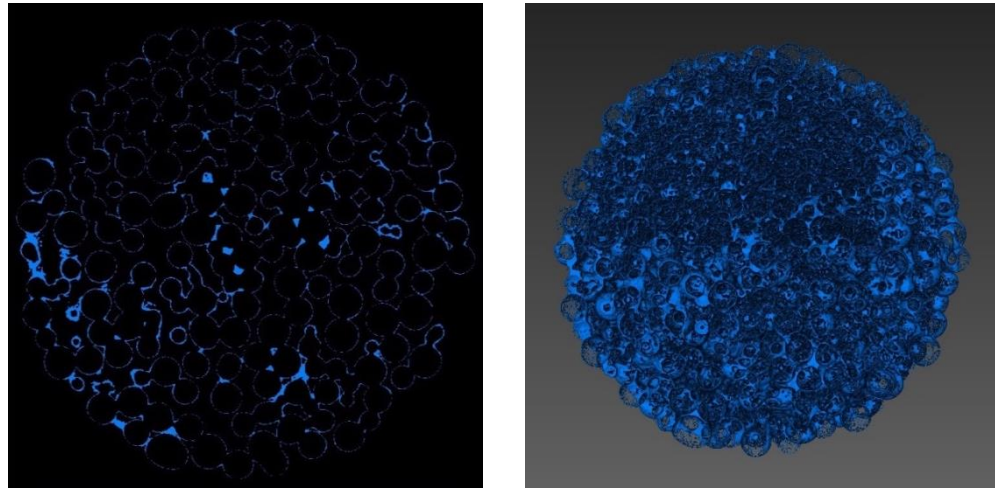


Figure 5.2.2.1 2D and 3D views of liquid phase in specimen I.

After calculating the volume fraction of the segmented liquid phase over the total scanned area, the saturation degree for each specimen was estimated and is listed in Table 5.2.2.2. Compared to the target saturation degrees, slightly higher values were determined using this method. Results confirmed that, for an unsaturated material, the saturation degree in the pendular regime might have a very limited range. Figure 5.2.2.2 and Figure 5.2.2.3 present both 2D and 3D views of specimen II and specimen III. The liquid phases were highlighted in blue. By comparing the 3D views between specimens with different saturation degrees, it could be found that a larger amount of liquid was developed to surround the particles when larger saturation degree was generated.

Table 5.2.2.2 Estimated saturation degrees by image processing.

	Volume of Pore Space (μm)	Volume of Liquid Phase (μm)	Saturation Degree
Specimen I ($Sr_t=6\%$)	7.65E+09	1.19E+11	6.44E-02
Specimen II ($Sr_t=9\%$)	1.08E+10	1.11E+11	9.77E-02
Specimen III ($Sr_t=12\%$)	1.37E+10	1.11E+11	1.23E-01

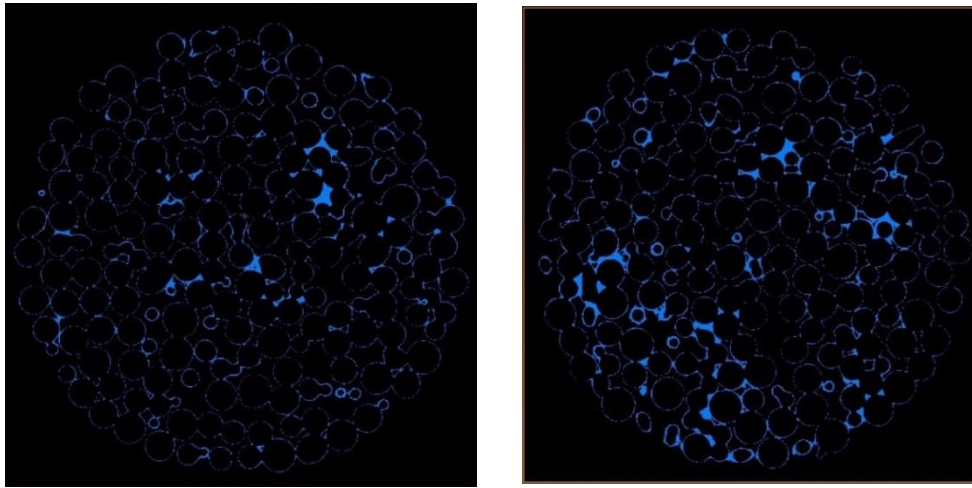


Figure 5.2.2.2 2D views of segmented liquid phase in specimen II and specimen III.

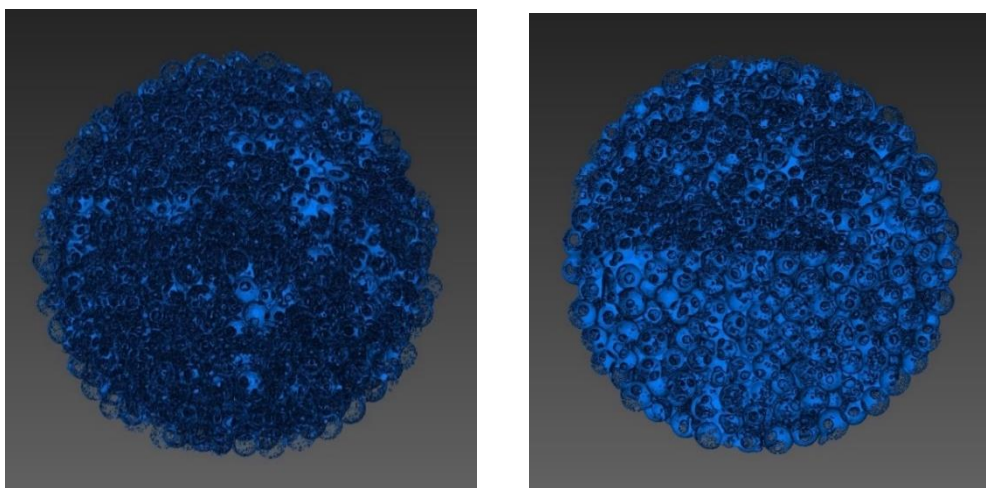


Figure 5.2.2.3 3D views of segmented liquid phase for specimens II and III.

To investigate the spatial distribution of the liquid phase among the central area of the specimen, the image slices were later cropped into the same cubic shape (Figure 5.2.2.4). The whole group of 601 image slices, numbered from 0 to 600, had a length of 600 pixels. The lengths of the cropped specimen were thus configured as 600 pixels in all three directions. Figure 5.2.2.4 also shows the xy plane of the liquid phase and the pore space in the cropped specimen I ($n = 0.453, S_r = 6.44\%$). Comparing the liquid phase and the pore space, it could be found that most liquid phase stayed around the glass beads although the particles had a relatively loose packing.

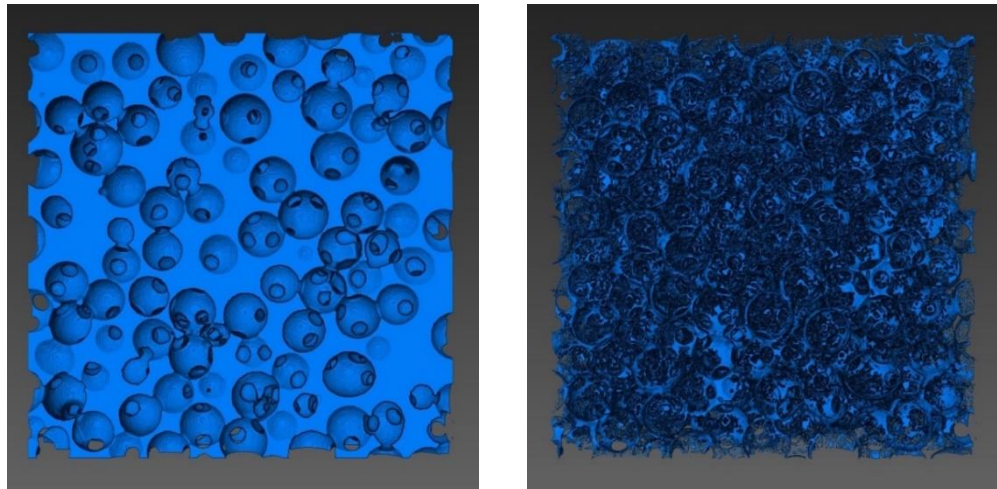


Figure 5.2.2.4 Pore space and liquid phase in the cropped specimen I ($n = 0.453, S_r = 6.44\%$).

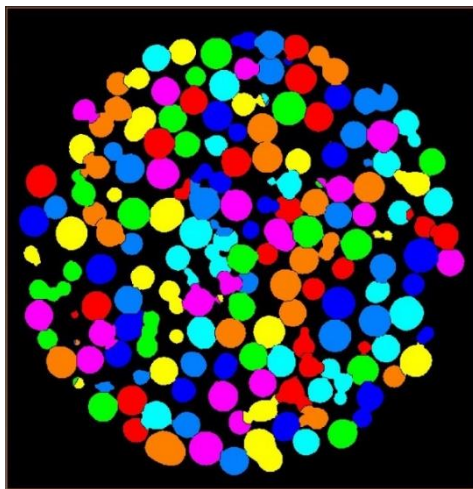
The saturation degree inside the cropped volume was also calculated and is listed in Table 5.2.2.3 for each specimen. In each assembly, a larger value of saturation degree could be found in the cropped region compared to that at the edges. This could be a consequence of the compression test conducted before the scan. Rather than distributed uniformly, more water migrates to the central area of the specimen. Results also show that the difference of saturation degrees between the cropped areas and edge areas increases when higher saturation degree.

Table 5.2.2.3 Estimated saturation degrees for cropped specimens.

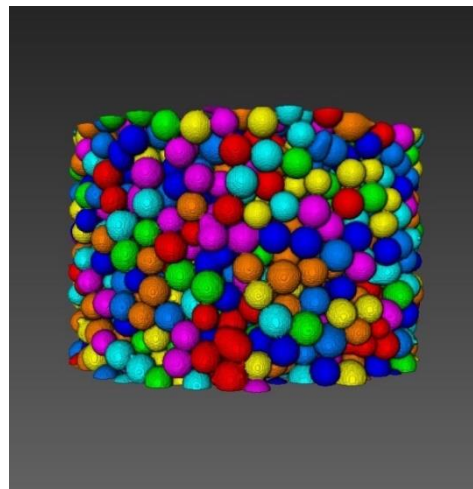
	Volume of Pore Space (μm^3)	Volume of Liquid Phase (μm^3)	Saturation Degree
Specimen I cropped	3.63E+09	4.82E+10	7.54%
Specimen II cropped	1.81E+09	1.51E+10	12.0%
Specimen III cropped	7.25E+09	4.45E+10	16.3%

5.2.3 Particle Phase and Particle Size Distribution

By using the watershed algorithm introduced in chapter 3, the binary images of glass beads could be separated and labelled with different colors. Figure 5.2.3.1 presents the segmented glass beads in specimen I ($n = 0.453, Sr = 6.44\%$).



(a) 2D view in the xy plan

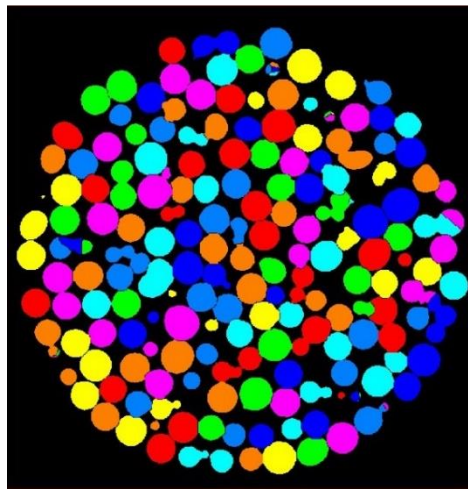


(b) 3D view in the xz plan

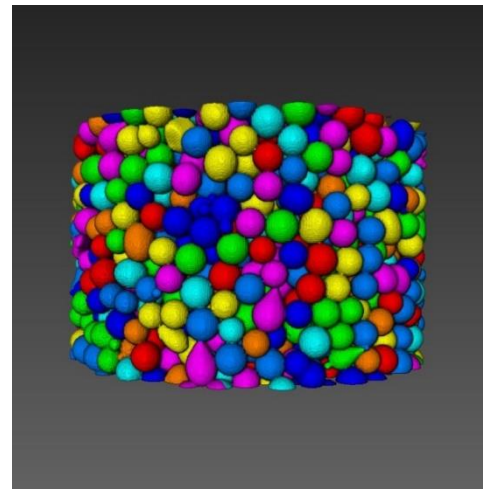
Figure 5.2.3.1 Glass beads segmented and labelled in specimen I.

Figure 5.2.3.2 and Figure 5.2.3.3 show the results for specimens II ($n = 0.425, Sr = 9.77\%$) and III ($n = 0.425, Sr = 12.32\%$). Similar results could be observed in the 2D images. It also could be found in all the 3D views that

most glass beads were spheres, however a few particles with random shapes could still be found among the three specimens.

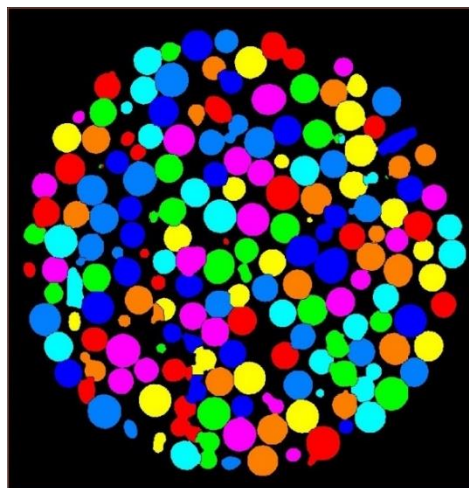


(a) 2D view in the xy plan

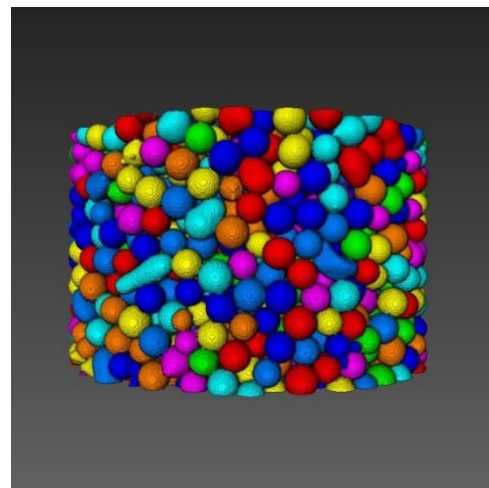


(b) 3D view in the xz plan

Figure 5.2.3.2 Glass beads segmented and labelled in specimen II.



(a) 2D view in the xy plan



(b) 3D view in the xz plan

Figure 5.2.3.3 Glass beads segmented and labelled in specimen III.

It could be found in the 2D image that most connecting particles were successfully segmented, although a small number of particle pairs or groups could still be observed. After labeling all the segmented glass beads, analysis of the labelled phase was carried out to calculate the particle number, and the particle

size for each segmented unit. Table 5.2.3.1 listed the calculated particle numbers, along with other previously estimated parameters for all three specimens.

Table 5.2.3.1 Estimated particle numbers for sample specimens.

	Porosity	Saturation degree	Particle number
Specimen I ($n = 0.453, Sr = 6.44\%$)	0.453	0.0644	1856
Specimen II ($n = 0.425, Sr = 9.77\%$)	0.425	0.0977	1981
Specimen III ($n = 0.425, Sr = 12.32\%$)	0.424	0.123	1964

Around 2000 particles were found in the analysis zone after the first and last 200 images were removed to achieve better resolution. It also could be found that the estimated particle number was inversely proportional to the porosity calculated earlier. For specimen II and specimen III that have almost identical porosities, similar particle numbers were also generated. However a smaller particle number was detected in specimen III, compared to specimen II which had a slightly larger porosity. This could result from the difference in the particle size distribution of the sample glass beads. To investigate the particle size distribution (PSD) of the glass beads in each sample specimen, PSD curves were plotted and are displayed in Figure 5.2.3.4.

Almost identical size distributions of the glass beads could be observed among all three specimens. The particle size was also determined within the range of fine sand and medium sand. For specimens II and III which had nearly-identical

particle numbers and porosities, slight difference could be found between their PSD curves.

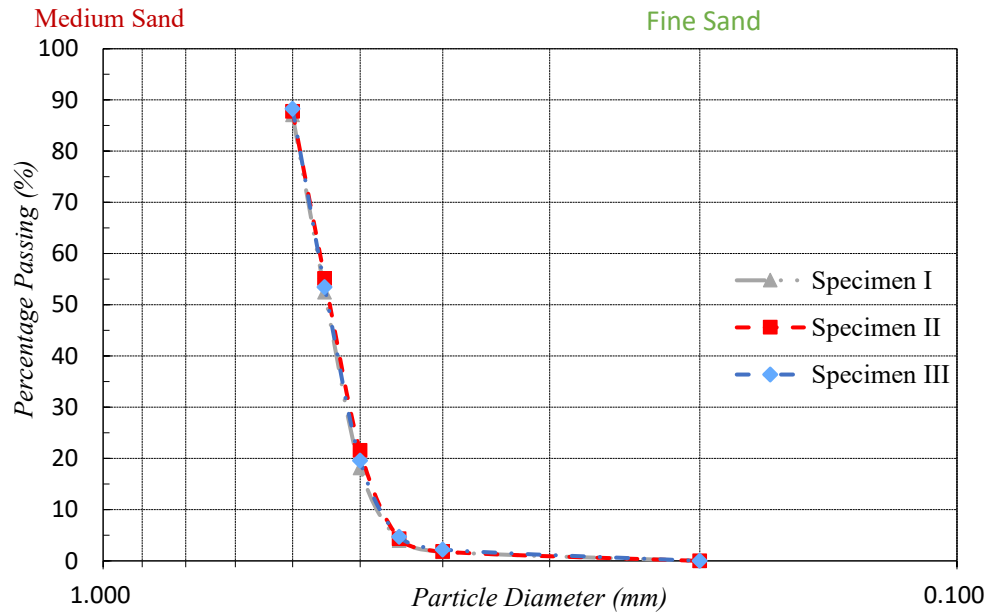


Figure 5.2.3.4 Estimated particle size distribution (PSD) curves for the experimental specimens.

5.2.4 Discussion

Three different phases (air, water, particle) of the unsaturated specimens were firstly segmented using image thresholding. A constant value of porosity was imposed on all three specimens with a series of target saturation degrees ($Sr_t = 6\%, 9\%, 12\%$). The total mass and the total volume of each unsaturated specimen were measured and controlled to achieve a similar porosity. After segmenting the pore space, the estimated porosities were found to be close to the target value of 0.43. Relatively larger porosity was generated in specimen I with lower saturation degree. The smaller porosity in specimen II and III were considered as a result of the increased cohesive capillary effects.

Secondly, the saturation degree in each specimen was determined by calculating the volume fraction between the liquid phase and the pore space. To compare to the DEM model, image slices for three specimens were cropped into the same cubic shape. Results in Table 5.2.2.2 showed that larger values of saturation degrees also could be found in the cropped areas when compared to the removed edge areas. This might result from the compression process conducted before the x-ray scan. Due to the compression, more water could migrate into the central area of the specimen rather than distributing uniformly. Due to the increasing capillary effects, results also showed that more water tended to gather within the central areas when higher saturation degrees were imposed.

The particle phase in each specimen was thirdly segmented using image thresholding. To investigate the particle number and the particle size distribution, the watershed algorithm was then applied to separate the contacting particles. Around 1900 particles were found within the analysis area for all three specimens. A relatively smaller number of particles were generated in specimen I as a larger porosity was produced earlier. It was also interesting to note that smaller particle number was detected in specimen III, compared to specimen II which had a slightly larger porosity. Particle size distributions were then investigated. Small difference could be found between the PSD curves of specimens II and III, which could explain the larger particle number in specimen II. Moreover, the size distribution of the glass beads was considered within the range between fine sand and medium sand.

5.3 Analysis of Liquid Phase

5.3.1 Number of Liquid Contacts

To analyse the number of capillary bridges and liquid clusters, a set of filters were used to remove the surrounding water. Since the sizes of both bridges and clusters could be reduced while the filtering was carried out, an overestimated liquid phase was segmented to prevent the removal of some capillary bridges that had small sizes during the process of filtering. Figure 5.3.1.1a shows the segmented liquid phase with overestimation for specimen I ($n = 0.453, Sr = 6.44\%$). Capillary bridges with bigger sizes could be found in the graph, as well as liquid clusters and liquid films.

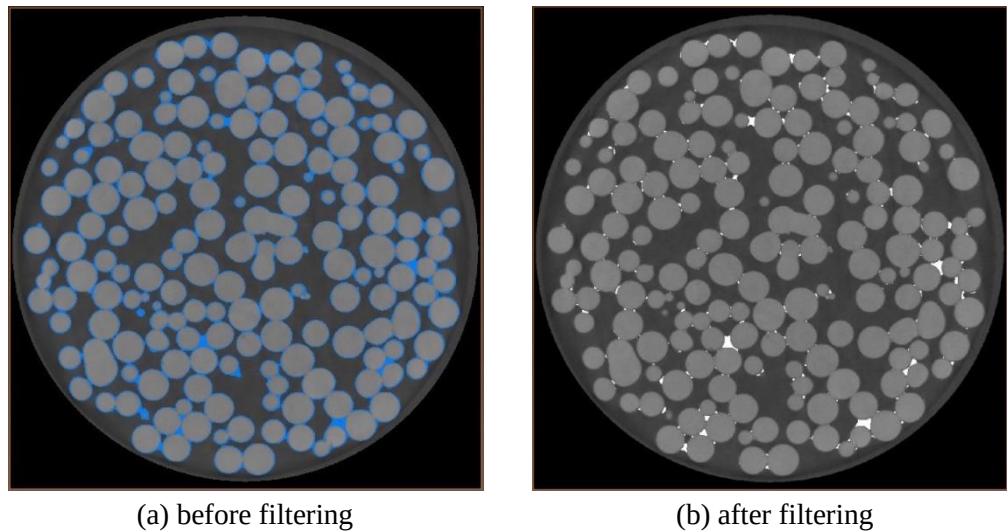
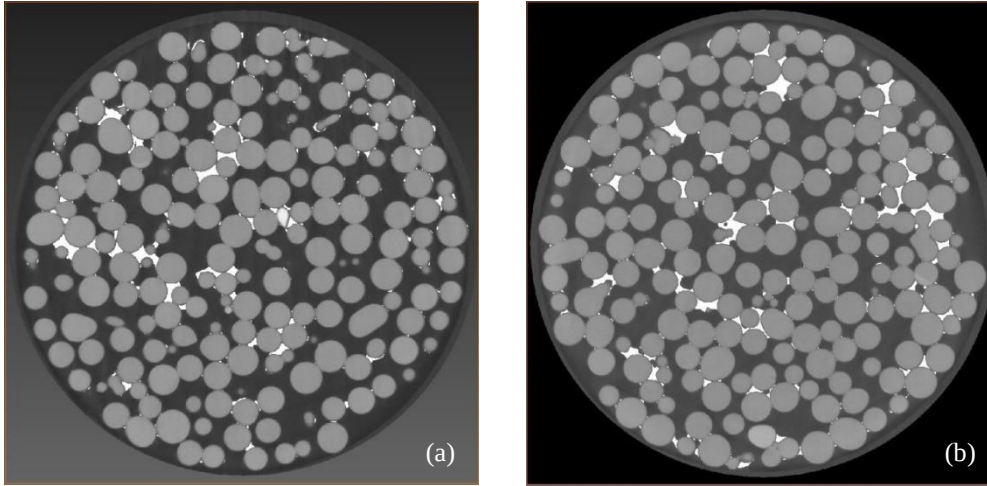


Figure 5.3.1.1 Liquid phase in specimen I, before and after filtering.

After applying a set of different filters liquid films surrounding particles could be removed; capillary bridges and liquid clusters remained and are highlighted in Figure 5.3.2.1b. Similarly, Figure 5.3.1.2 shows the 2D views of filtered liquid phases for specimens II ($n = 0.425, Sr = 9.78\%$) and III ($n = 0.424, Sr = 12.34\%$) in the xy plane.



(a) specimen II ($n = 0.425, Sr = 9.78\%$), (b) specimen III ($n = 0.424, Sr = 12.34\%$)

Figure 5.3.1.2 Liquid contacts highlighted in specimen II and III.

It could be observed in filtered images that almost no presence of water films could be detected after the liquid phase was filtered. All the liquid clusters remained although changes occurred in their shapes and sizes. The change in size could be neglected in this case since the aim here focused on determining the number of liquid contacts. A few bits of remaining water could still be found surrounding the particles. This could lead to a slightly overestimated number of capillary bridges.

Additionally, in the 2D views of the filtered liquid phases, two liquid contact points could be found at some particle-particle interfaces. The 3D view of the detail information for this type of contact is presented in Figure 5.3.1.3a. As shown in Figure 5.3.1.3b, for two particles that were in contact, a liquid ring could occur at the particle-particle interface. Since the contact areas between two particles were considered as unneglectable in practical problems, instead of forming capillary bridges, liquid rings would develop at the particle-particle contact interfaces. Therefore, it was assumed in this study that, when calculating

the total number of liquid contacts, a liquid ring was accounted as one contact as well as a capillary bridge and a liquid cluster.

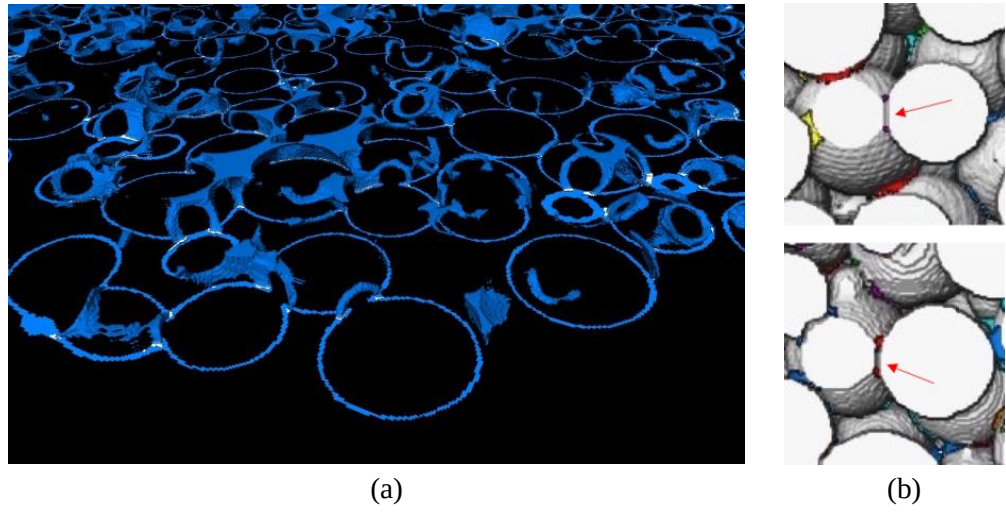
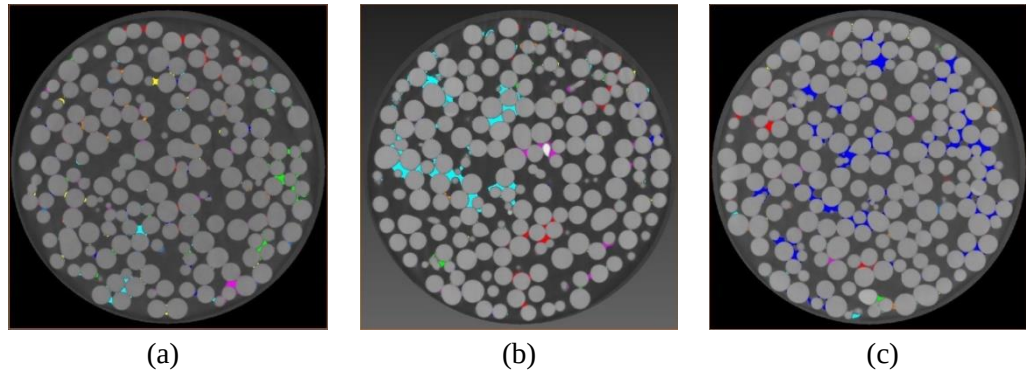


Figure 5.3.1.3 Liquid ring developed at particle-particle interface.



(a) specimen I ($n = 0.453, Sr = 6.44\%$), (b) specimen II ($n = 0.425, Sr = 9.78\%$), (c) specimen III ($n = 0.424, Sr = 12.34\%$).

Figure 5.3.1.4 Labelled liquid contacts for three specimens in the xy plane.

The total number of liquid contacts, including liquid ring, capillary bridge and liquid cluster was later determined by labelling the filtered liquid phase and calculating the number of labelled units. The 2D view (xy plane) of the labelled liquid contacts for specimen I ($n = 0.453, Sr = 6.44\%$) is presented in Figure 5.3.1.4a, overlaying the original 2D cross section images acquired from X-ray

CT. Disconnected bridges or clusters were labelled using various colours. Liquid rings on connecting particles could be found to be two dots with the same colour. Moreover, Figure 5.3.1.4b and Figure 5.3.1.4c present the 2D views of the labelled liquid contacts for specimen II and III in the xy plane. The estimated number liquid contacts for each specimen is listed in Table 5.3.1.1, with other parameters determined previously.

Table 5.3.1.1 Estimated parameters for sample specimens.

	Porosity	Saturation degree	Particle number	Number of liquid contacts
Specimen I ($n = 0.453, Sr = 6.44\%$)	0.453	0.0644	1856	9180
Specimen II ($n = 0.425, Sr = 9.78\%$)	0.425	0.0977	1981	11515
Specimen III ($n = 0.424, Sr = 12.34\%$)	0.424	0.123	1964	8891

In Table 5.3.1.1, the largest number of bridges and clusters could be observed in specimen II, where the greatest particle number was generated. Compared to specimen II, a slightly smaller number of bridges and clusters was detected in specimen III although a larger saturation degree was achieved. This could result from the increasing probability for the generation of liquid clusters when the saturation degree passed a certain limit. The gathering of capillary bridges could eventually lead to the development of liquid clusters. As liquid clusters could come from one or more capillary bridges, the increase in the number of liquid clusters thus might lead to a decrease in the number of both bridges and clusters.

5.3.2 Size Distribution of Liquid Contacts

After labelling and calculating the number of liquid contacts for each sample specimen, it was found that the number of liquid contacts increased firstly and then significantly decreased while raising the saturating degree. This was suspected to occur because of the increasing probability for the formation of connected liquid clusters when more water was involved. As a result, the total number of liquid contacts would decrease since several capillary bridges could emerge into a single liquid cluster. Investigations of the size distribution of the liquid contacts were then carried out to better understand the relation between saturation degree and number of liquid contacts.

Figure 5.3.2.1a presents a 3D view of labelled liquid contacts in specimen I ($\emptyset = 0.453, Sr_t = 6.44\%$). Figure 5.3.2.1b shows the cropped specimen with the labelled liquid contacts and the segmented particles. All three types of liquid contacts, including liquid films, capillary bridges and liquid clusters could be found in specimen I. It was interesting to note that some capillary bridges appeared to attach to more than two particles.

The unsaturated sample specimens in this study could be regarded as beyond the pendular regime, *i.e.* in the funicular regime. It was found that the ideal pendular regime could be challenging to achieve in practice as water was usually randomly distributed amongst the particles. The 3D reconstruction of the cross section images also revealed that some liquid contacts appeared to be connected although they could be observed as separated in the 2D view.

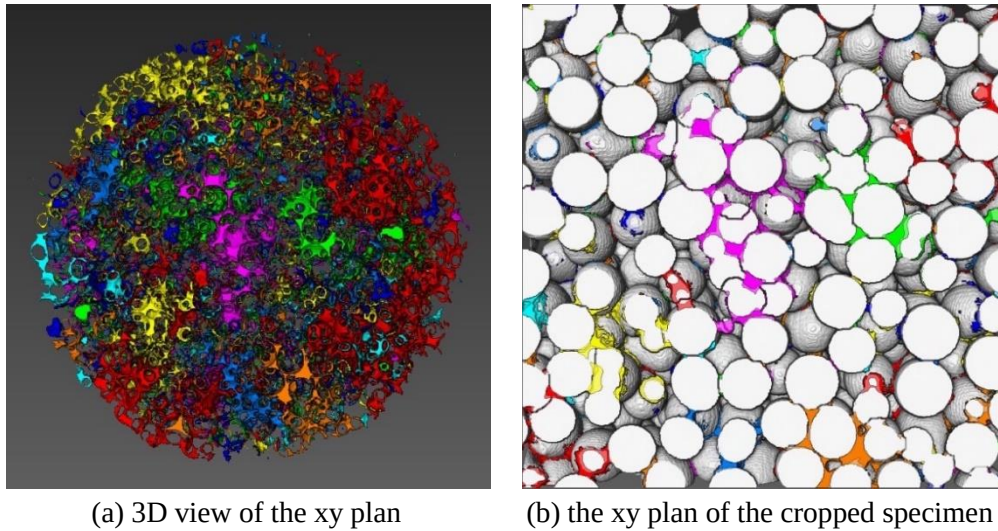


Figure 5.3.2.1 Labelled liquid contacts in specimen I.

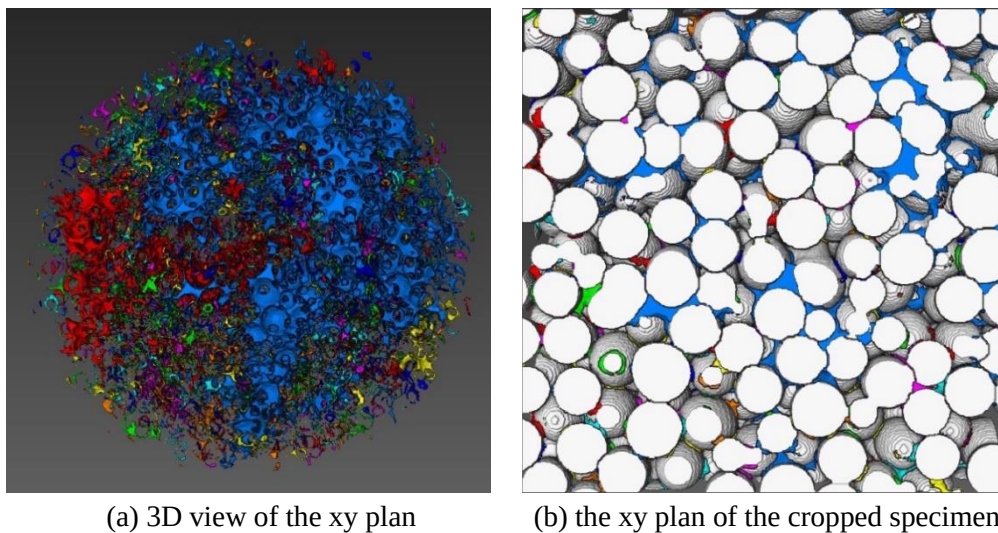


Figure 5.3.2.2 Labelled liquid contacts in specimen II.

Similarly, Figure 5.3.2.2 and Figure 5.3.2.3 present the labelled liquid contacts in specimens II and III respectively. Compared to specimen I that had the lowest saturation degree, more liquid clusters could be found in both specimens II and III. By comparing the 3D views between specimens II and III, liquid clusters with larger sizes could be found in specimen III where a larger saturation degree was generated. An analysis of the size distribution of liquid contacts was carried

out for verification purposes. Figure 5.3.2.4 demonstrates the size distribution of the three different types of liquid contacts.

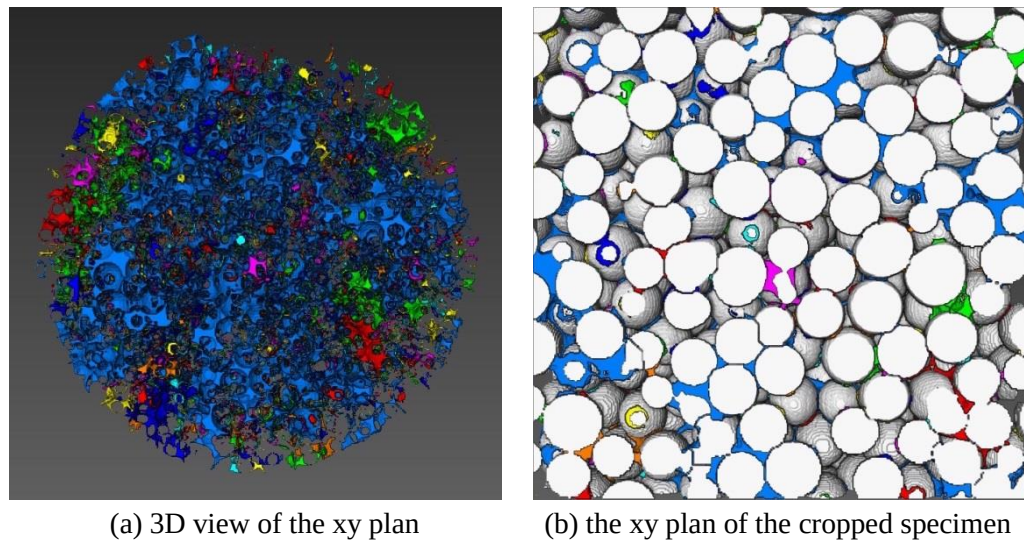


Figure 5.3.2.3 Labelled liquid contacts in specimen III.

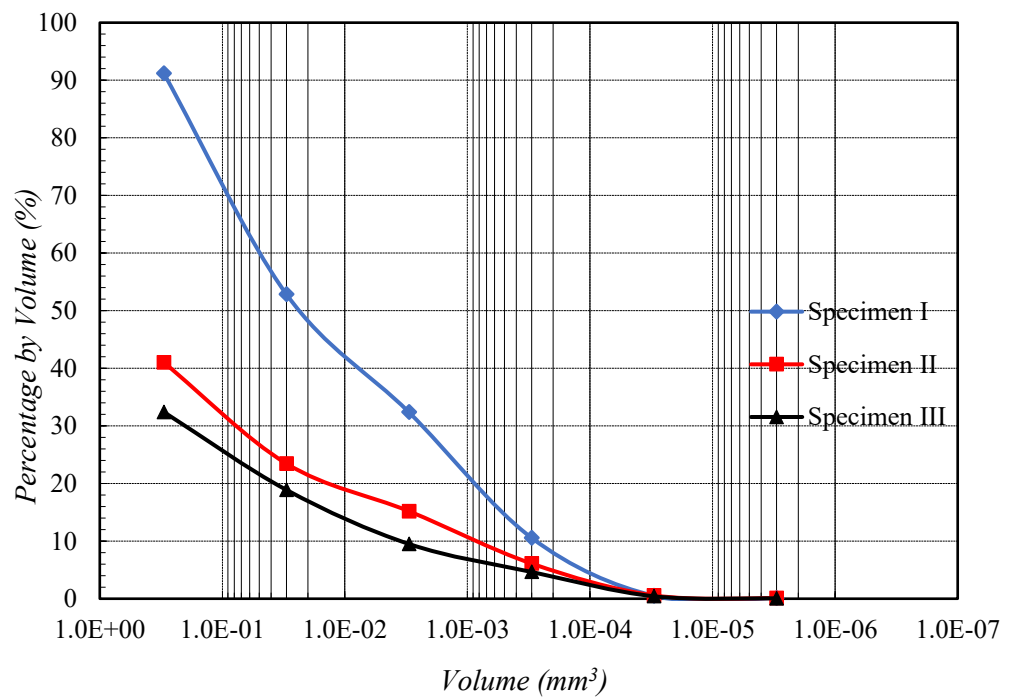


Figure 5.3.2.4 Size distribution of liquid rings, capillary bridges and liquid clusters.

It could be found from the figure above that the liquid contacts with the largest sizes were developed in specimen III, while specimen I had the smallest ones.

Compared to specimen I, similar size distribution curves could be found for specimen II and III. This shows that both these two specimens could have more liquid clusters than capillary bridges or liquid rings that connected only two particles. As estimated previously, the smallest number of liquid contacts could be found in specimen III, which had the highest saturation degree. This could also imply that a significant number of capillary bridges and liquid clusters would merge into each other and start to form connected ganglia when the saturation degree reached a certain limit. According to the results in this study, this limit for the saturation degree could be within the range from approximately 9% to around 12%. Whilst the saturation degree was controlled to be around 6%, more capillary bridges and liquid rings were generated, as much smaller size of liquid contacts could be found in specimen I.

5.3.3 Distribution of Saturation Degree

To investigate the distribution of the water phase and then incorporate this into the DEM method, the cropped image slices were broken down into 27 cubes for the analysis of saturation degrees in each cube unit.

Figure 5.3.3.1 illustrates the split plot for the cropped images. The whole image slices, numbered from 0 to 600, had a length of 600 pixels. The lengths of the whole cropped cube were thus configured as 600 pixels, and the lengths of all the cube units were set as 200 pixels. By calculating the volume fraction of the liquid phase over the pore space, the saturation degree could be obtained for each cube unit. The saturation degrees in each cube unit are listed in Figure 5.3.3.2.

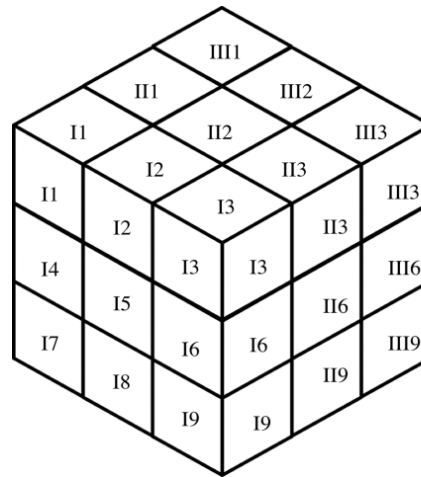


Figure 5.3.3.1 Image slices splitted for the determination of water distribution.

It could be observed in Figure 5.3.3.2 that a maximum value of saturation degree was found to be c. 13% for specimen I. Similarly, the maximum values for specimen II and III could be determined to be c. 20%, and 26% respectively (Figure 5.3.3.3). The largest standard deviation for the saturation degree was achieved in specimen III. It also could be found that the standard deviation for the saturation degree increased when the water content was raised. The largest range of the saturation degree, moreover could be found in specimen III to be c. 17.6%, while the smallest range was achieved in specimen I as c. 7.5%.

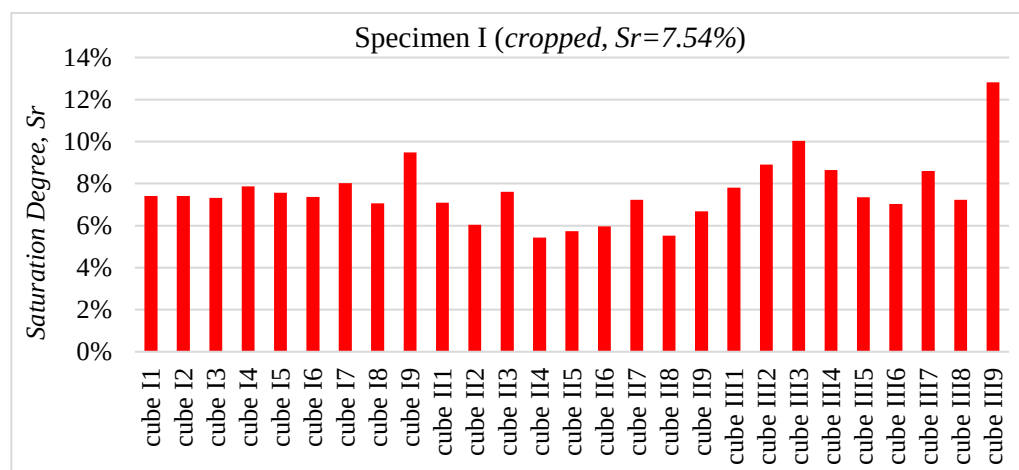
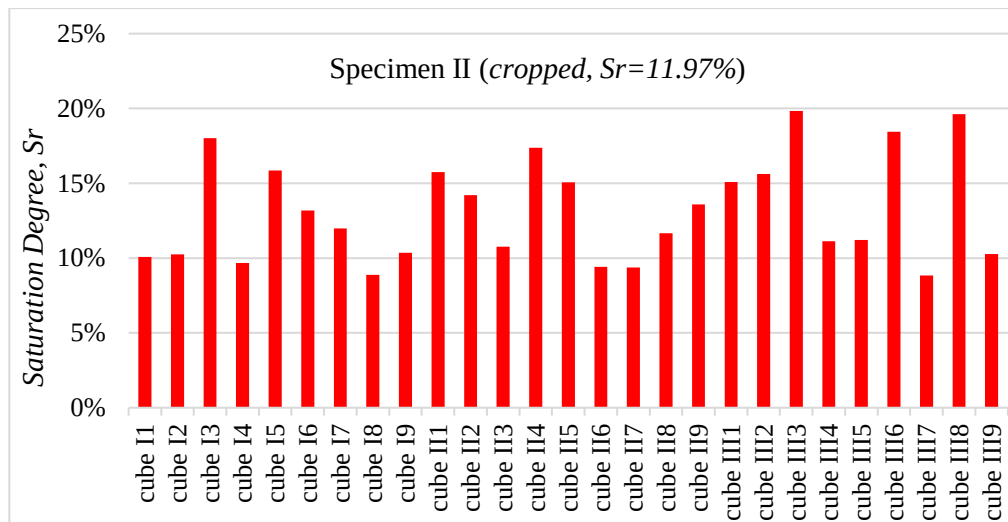
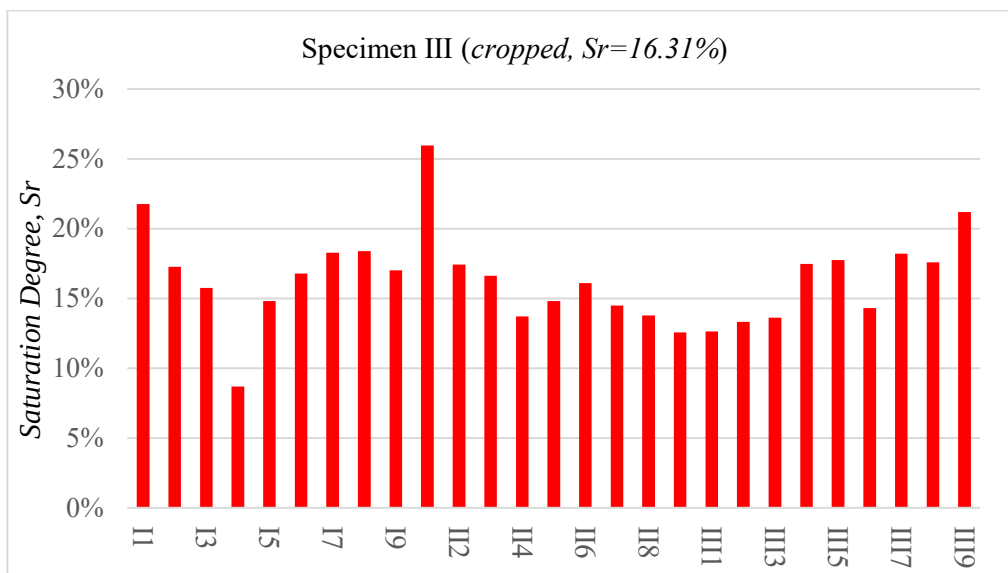


Figure 5.3.3.2 Distribution of saturation degree in cropped specimen I.



(a) specimen II.

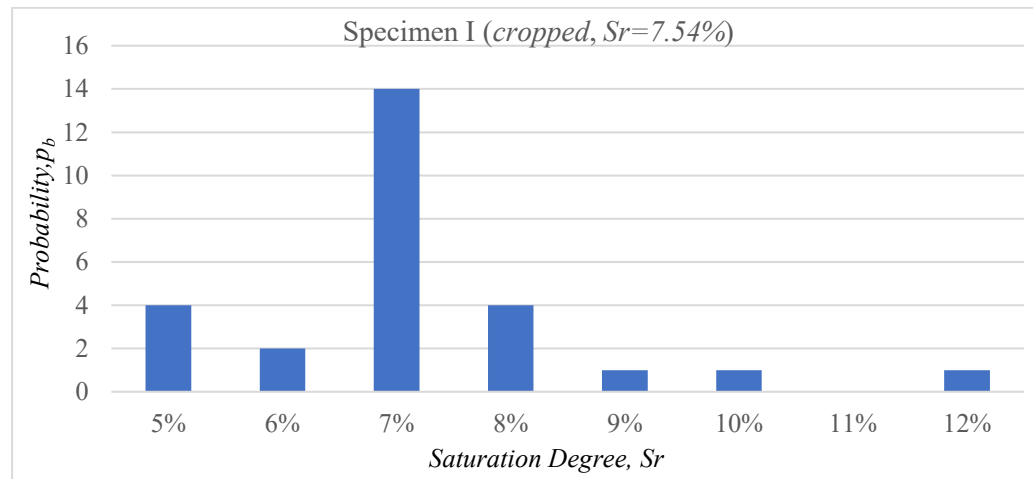


(b) specimen III

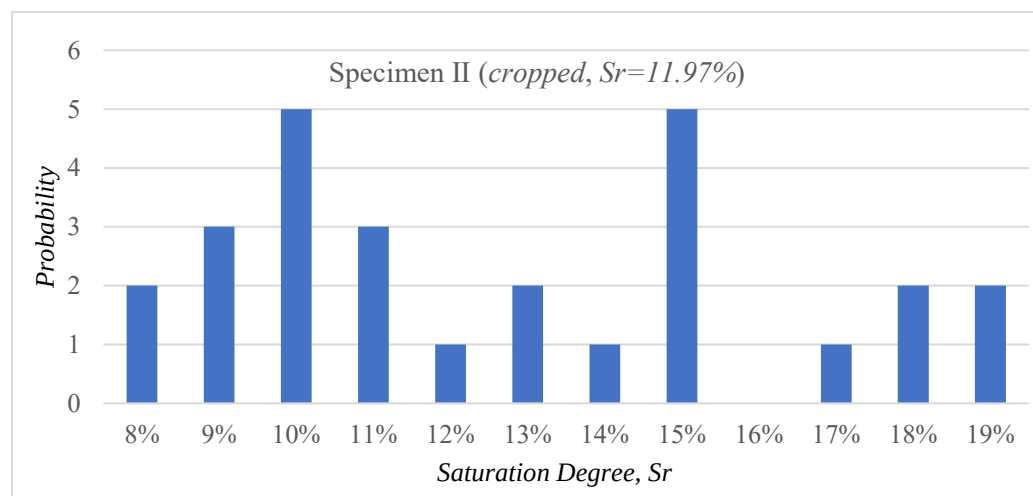
Figure 5.3.3.3 Distribution of saturation degree in cropped specimens II and III.

Figure 5.3.3.4 and Figure 5.3.3.5 show the probability of saturation degrees in each sample specimen. In specimen I, it could be found that the highest probability of saturation degree occurred within 7%-8%, which represents the average value of 7.54% (Figure 5.3.3.4a). However, two highest probability values could be found in specimen II, which were within 10%-11% and 15%-16% respectively. Both these ranges were different from the average value of

11.97% (11%-12%) which had the second highest probability (Figure 5.3.3.4b). In specimen III, moreover it could be determined that the highest probability of saturation degree occurred in 17%-18%, while the average value 16.31% (16%-17%) only had the third highest probability (Figure 5.3.3.5). The results above reveal that when a relatively higher saturation degree was generated in an unsaturated material, the liquid phase was more likely to be unevenly distributed and larger range of saturation degrees could be developed. Thus, it might be insufficient to apply an average value of saturation degree, *e.g.* a constant value of matric suction, in an unsaturated DEM model.



(a) specimen I



(b) specimen II

Figure 5.3.3.4 Probability of saturation degree in cropped specimens I and II.

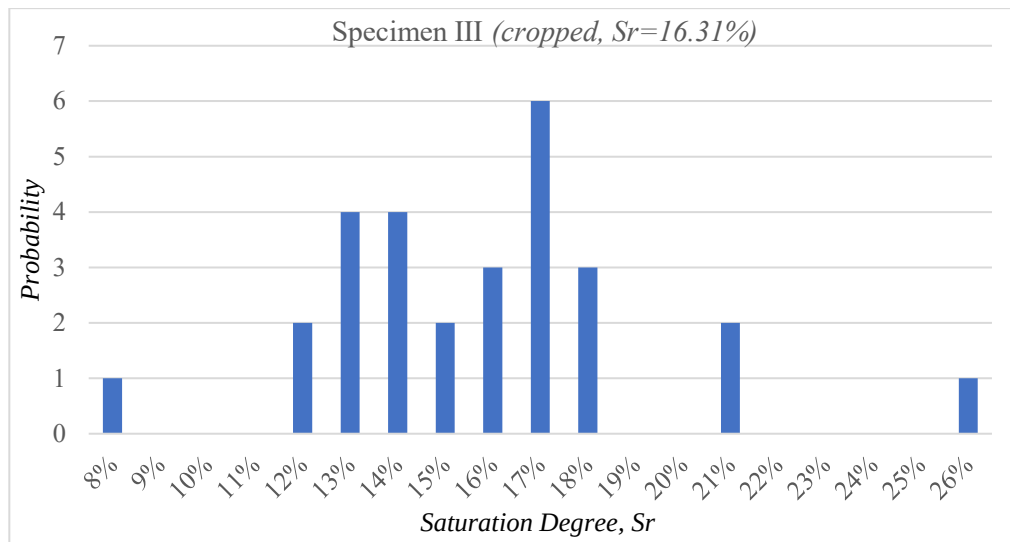


Figure 5.3.3.5 Probability of saturation degree in cropped specimen III.

5.3.4 Discussion

Since the water was imposed as uniformly distributed as possible, liquid films were found to be surrounding every particle. After applying a series of image filters with various parameters, the liquid phase could be reduced to where only liquid contacts remained. Three forms of liquid contacts are considered in this study. They consist of the capillary bridge, the liquid cluster and the liquid ring which appeared to generate between two contacting particles. It was found that the largest number of liquid contacts (11515) occurred in specimen II, where a saturation degree of approximately 9.77% was imposed. It could also be observed that the smallest number of liquid contacts (8891) was determined in specimen III which had the highest saturation degree of around 12.34%. Around 9180 liquid contact, moreover was found in specimen I ($Sr = 6.44\%$). Size distribution for the liquid contacts in each specimen was then plotted (Figure 5.3.2.4). It could be observed that the liquid contacts with the largest sizes were generated in specimen III, while the smallest ones could be found in specimen I.

These observations may imply that a significant number of capillary bridges and liquid clusters would migrate into each other and form connected liquid ganglia when the saturation degree reaches a critical limit. The results appear suggest that this limit for the saturation degree could be within the range from approximately 6% to 12%. The strength of an unsaturated material may decrease significantly when the saturation degree exceeds this critical point. Moreover, the appearance of liquid clusters in the specimens with relatively low saturation degree may indicate that it is irrational to use only capillary bridges in DEM.

The distribution of the liquid phase in each specimen was later investigated by analysing the distribution of saturation degrees. By calculating the standard deviation, and the probability of occurrence of the saturation degree value, results were presented in Figures 5.3.3.2 and 5.3.3.3. In specimen I, the highest probability of occurrence of saturation degree was found to be identical to the average value of 7.54%. However, the average saturation degree of 11.97% was detected as the second highest probability in specimen II. The two highest probability values were determined to be within 10%-11% and 15%-16% respectively. In specimen III, moreover it could be determined that the highest probability of saturation degree occurred in 17%-18%, while the average value only had the third highest probability. The results thus suggest that when a relatively higher saturation degree is imposed in an unsaturated material, the liquid phase would be more likely to unevenly distribute, and a larger range of saturation degrees could then be developed. Therefore, it may be insufficient to only consider the average value of saturation degree when dealing with unsaturated materials in practice.

Moreover, since water distribution is strongly dependent on the sample preparation. Water phase may be more evenly distributed if the specimen can be dried from a fully saturated state to a desired degree of saturation. Although it might be difficult to accurately control the desired saturation degree with this method.

5.4 Geometry of Capillary Bridge

5.4.1 General Geometry

As previously shown in chapter 3, capillary bridges were commonly assumed as symmetrical to the axis that passed through the centroids of two adjacent particles. However, many capillary bridges with inconstant curvature could be found among all three sample specimens.

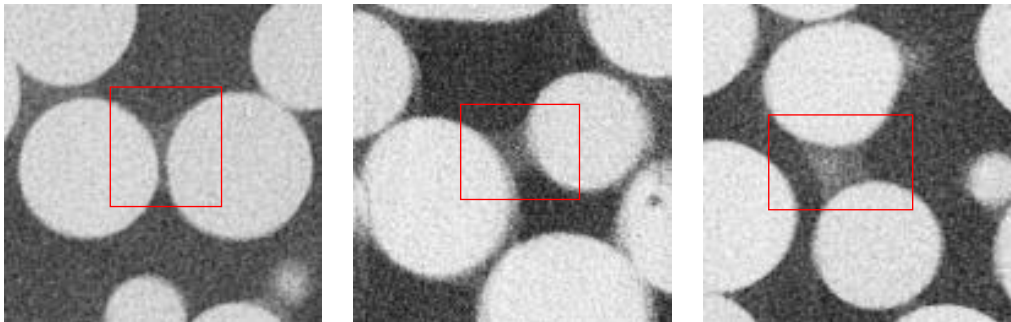


Figure 5.4.1.1 Capillary bridges with inconstant curvature.

Figure 5.4.1.1 presents examples of unsymmetrical capillary bridges. It could be seen in such circumstances that capillary bridges depart significantly from the axis which passes through the particle centroids. It also could be observed that these capillary bridges are not symmetric figures as commonly assumed. The imperfection of sample grains could be one of the factors leading to this phenomenon. It also indirectly confirmed that in practical terms, capillary

bridges could develop between two grains without being located symmetrically to the axis that passes through the grain centroids.

These phenomena were found to contradict the toroidal approximation method which was used for estimating the capillary bridge geometry. This numerical model assumes that the average meniscus curvature is identical at all locations over the air-liquid interface. It suggests that, for two adjacent grains with a given interparticle distance, the same meniscus curvature would be generated with a specific value of the saturation degree. The results of this study however reveal that capillary bridges with inconstant curvature could develop between two solid grains without locating symmetrically to the axis passing through the particle centroids (Figure 5.4.1.1).

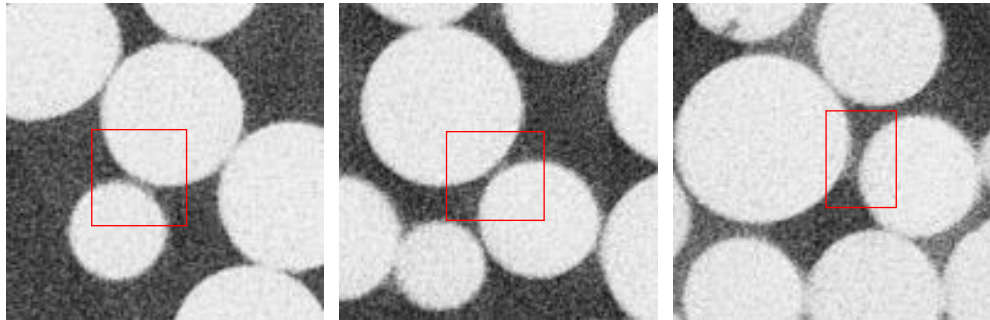


Figure 5.4.1.2 Capillary bridges with predominantly concave menisci.

Figure 5.4.1.2 shows capillary bridges with very similar meniscus curvature, and which comply with the assumption in the numerical model. Predominantly concave menisci also could be found here. 3D images for a concave capillary bridge are also presented in Figure 5.4.1.3. In such circumstances, the internal radii of the capillary bridges were determined to be larger than the external radii. According to the Gorge method (Equation 3.1.2), capillary forces here could be

determined by calculating the sum of the pressure difference applying at the bridge neck and the water surface tension on the air-liquid interface.

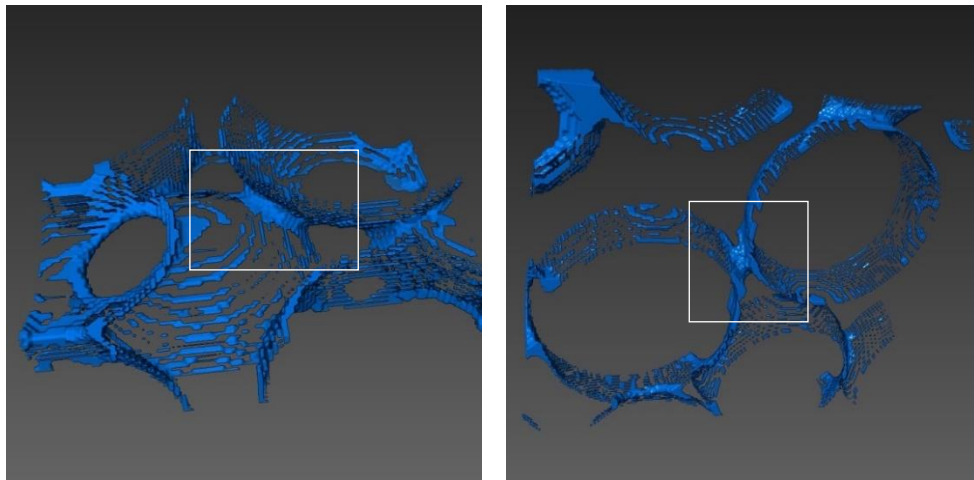


Figure 5.4.1.3 3D views of a capillary bridge with predominantly concave menisci.

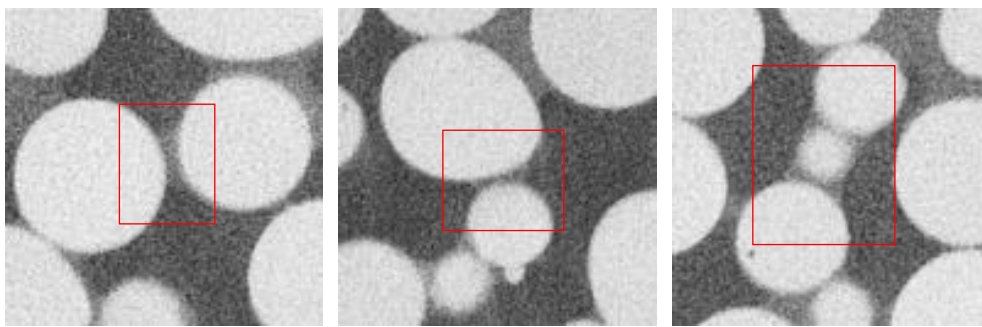


Figure 5.4.1.4 Capillary bridges with predominantly convex menisci.

Furthermore, capillary bridges with predominantly convex menisci also could be found for unsaturated specimens with spherical glass beads at low water content (Figure 5.4.1.4). Predominantly convex menisci could be found in these circumstances. More occurrence of this type of capillary bridge could be observed when higher saturation degrees were imposed. To understand the differences of mechanism in capillary bridges with predominantly concave and convex menisci, Figure 5.4.1.5a and Figure 5.4.1.5b present the difference between these two types of capillary bridge using their schematic illustrations at the contacts between two idealised spherical particles. The forces exerted by the

capillary bridge with predominantly concave or convex menisci are also illustrated in the figure below.

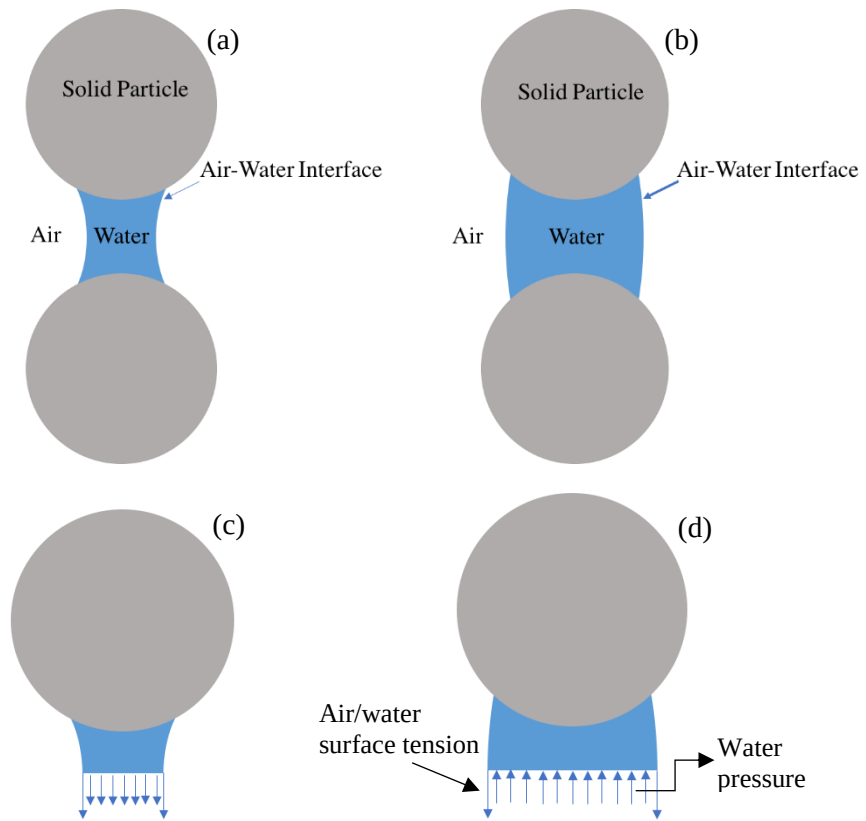


Figure 5.4.1.5 Illustrations of capillary bridges with predominantly concave and convex menisci.

In Figure 5.4.1.5c, it can be observed that the water pressure is commonly considered to be tensile in the predominantly concave menisci, bonding neighbour particles. However, the water pressure could be developed at the opposite direction and may generate compressive force on particles if predominantly convex menisci are generated (Figure 5.4.1.5d). Since the surface tension acting inside the contractile skin pulls the particles together, both compressive and tensile force may be generated on each particle due to the occurrence of predominantly convex menisci. In this case, the direction of force

depends on the relative magnitudes of water pressure and air-water surface tension.

5.4.2 Investigation of Matric Suction

Figure 5.4.2.1 shows the capillary bridges that had larger external radii than their internal radii. In such circumstances, capillary bridges were found between glass beads with relatively longer inter-particle distance. The difference between the external and internal radii was found to be opposite to the general assumptions for capillary bridges with predominantly concave shapes. According to the Young-Laplace equation, this could lead to negative values of matric suction and capillary force. Repulsive forces thus were generated in these circumstances, acting through the capillary bridge between two adjacent particles. It was interesting to note that a capillary bridge with almost flat menisci was generated in Figure 5.4.2.1c. The external radius of the capillary bridge could be regarded as approaching infinity in this case. This may indicate that the repulsive forces between the solid particles could eventually become an important reason for the increasing strength of an unsaturated material.

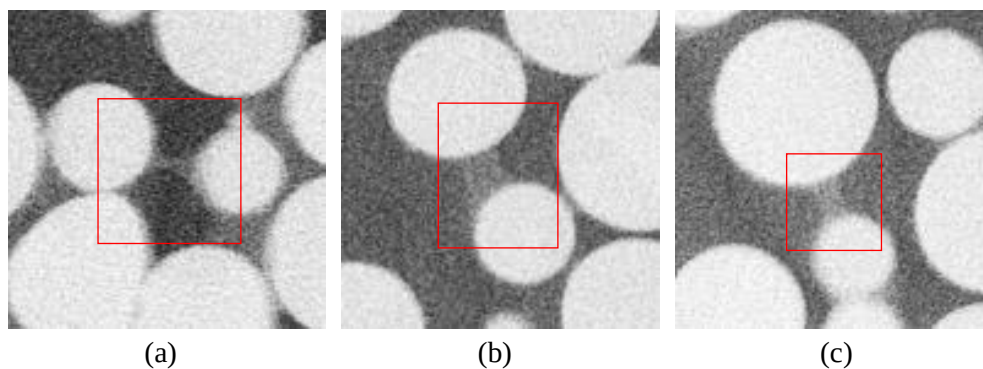


Figure 5.4.2.1 Capillary bridges with larger external radii.

Figure 5.4.2.2 demonstrates that different values of contact angle were generated with capillary bridges on the same glass bead. It was found in this study that,

contact angles would vary in an unsaturated specimen that consisted of only spherical particles. A larger contact angle was more likely to occur between two glass beads with longer inter-particle distance. It was also found that capillary bridges with longer interparticle distance were more likely to form when higher saturation degree was imposed. Therefore, the range of the contact angles could be raised due to the increasing saturation degree. In practical terms, the values of matric suction in an unsaturated material could vary significantly even when the liquid phase is considered as uniformly distributed. The results here thus, suggest that there might be another limitation of the capillary bridge model, where only the contact angle could be imposed.

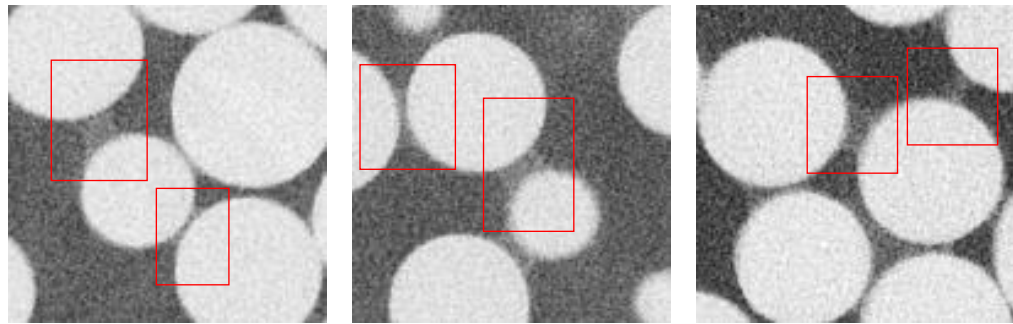


Figure 5.4.2.2 Various contact angles of capillary bridges.

5.4.3 Formation of Liquid Ring

As described previously, a liquid ring would surround the particle-particle interface when a pair of particles are in contact. Figure 5.4.3.1a showed the formation of liquid rings. In the 2D view, a liquid ring was marked by two white dots located beside the particle-particle interface. In Figure 5.4.3.1b, the 3D view of the liquid phase shows that glass beads were grouped together due to the appearance of liquid rings. It could be found that the contact area between two

connecting particles thus could be influential for determining the volume of capillary bridges.

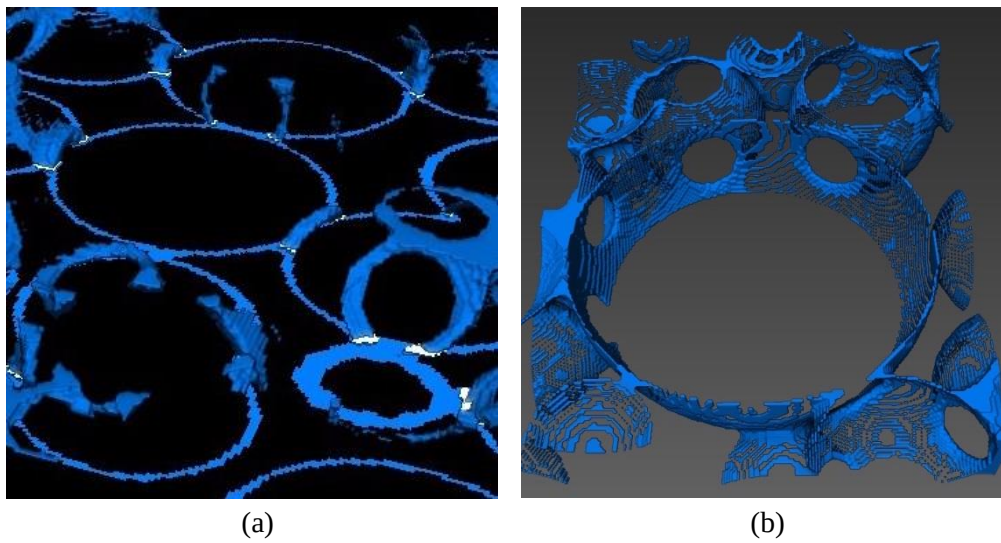


Figure 5.4.3.1 Liquid rings formed at particle-particle interfaces.

It was interesting to note that the above results contradicted the capillary bridge model in the DEM method for two connecting particles. The toroidal approximation method assumes that capillary bridges would generate as usual when two particles are in contact. Since the contact area between two contacting particles was neglected, the numerical modelling results showed that capillary bridges with the largest volume would be produced when two spherical grains were in contact. However, for two contacting particles, the results from this study reveal the development of liquid rings instead of capillary bridges.

Compared to an ideal capillary bridge generated at the particle-particle interface, smaller volumes would be developed for a liquid ring. For two particles with a certain matrix suction, whilst increasing the inter-particle distance, the volume of a capillary bridge therefore might increase firstly before starting to decrease.

The largest volume of capillary bridge could be achieved when two particles just start to separate. Figure 5.4.3.2 demonstrates the 3D view of both a liquid ring and a capillary bridge formed at the same glass bead. These images show that a larger volume was achieved here by the capillary bridge, when the particles were apart from each other.

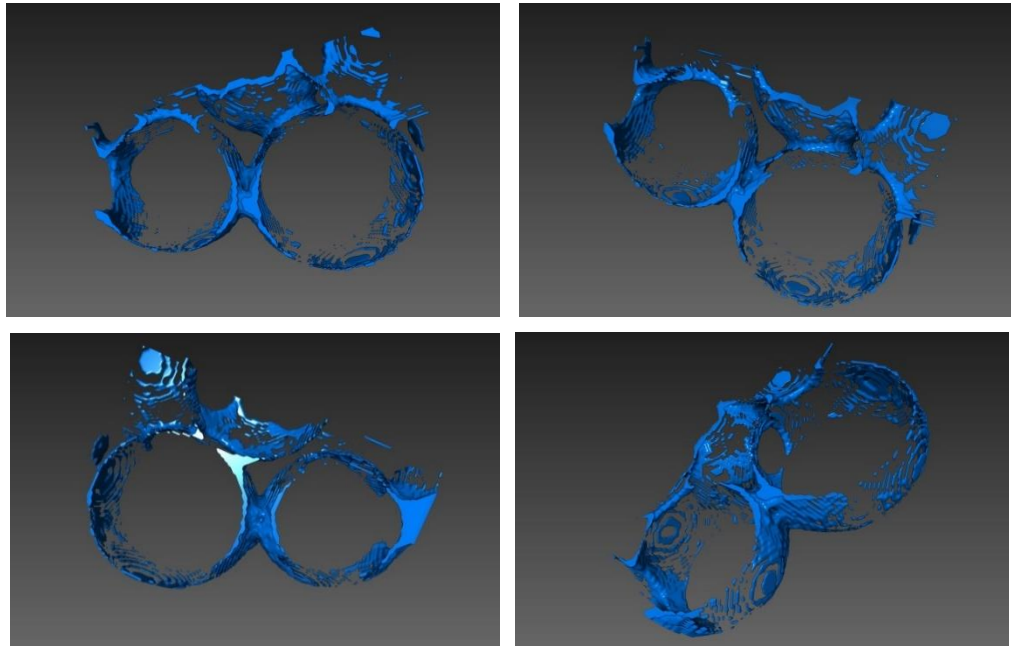


Figure 5.4.3.2 Capillary bridge and liquid ring formed at the same glass bead.

Based on the contact law proposed by Wang (2014), Figure 5.4.3.3 presents the contact law of the capillary bridge in the numerical model with the consideration of the liquid ring formation. Firstly, the contact force would gradually decrease to zero when the overlap distance is increased. The blue dash-dotted lines represent the evolution of contact force with Hooke contact and Hertz contact after the contact (Wang, 2014). When the liquid ring is formed at the particle-particle interface, a sudden reduction in the contact force would occur when these particles get in contact. Different values of the maximum contact force could be developed in these cases.

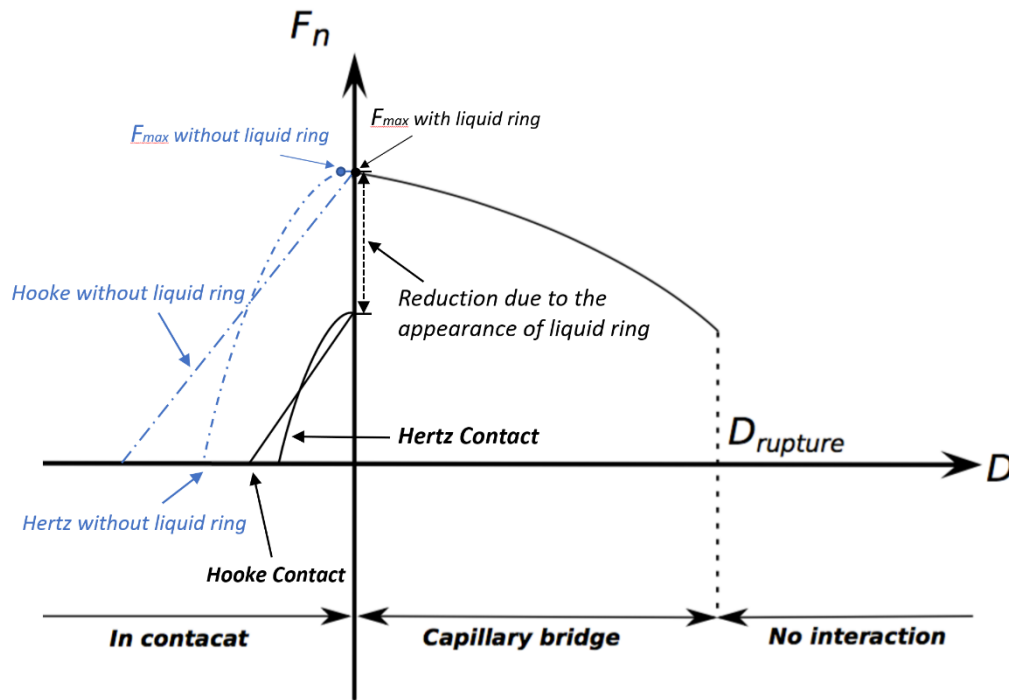


Figure 5.4.3.3 Contact law of capillary bridge with the appearance of liquid ring.

5.4.4 Discussion

Since osmotic is commonly neglected in this study, the matric suction would coincide with the total suction of an unsaturated material. The numerical model suggests that, for two adjacent grains with a given interparticle distance, the same meniscus curvature would be generated with each imposed value of saturation degree. However, a number of capillary bridges could be found to comply with this general assumption in this study (Figure 5.4.1.2). According to the Gorge method (Equation 3.1.2), the capillary forces in such circumstances can be calculated by the sum of the pressure difference acting on the bridge neck and the water surface tension on the air-liquid interface. However capillary bridges with asymmetrical menisci could also be found amongst all three unsaturated specimens (Figure 5.4.1.1). The observations may imply that capillary bridges could present an asymmetrical shape with inconstant meniscus

curvature, and without locating symmetrically to the axis passing through the particle centroids. It contradicts the numerical model which neglects the influence of the gravity and assumes that the average meniscus curvature is identical at any point over the air-liquid interface. Since only 2D cross sections were obtained, imperfections of the particles could be one of the factors leading to this phenomenon. It may also suggest that the specimen was not at equilibrium during the X-ray CT and some creep occurred.

Since the particle-particle interface is usually neglected in both theoretical and numerical analysis when considering only spherical particles, it is usually assumed that capillary bridges could form between two contacting particles. The numerical modelling results moreover indicate that the largest volume of capillary bridges is achieved when two particles are in contact. However, the observations from this study suggest a liquid ring would generate at the particle-particle interface (Figure 5.4.3.1). Since the interface area for two contacting particles may not be ignored in practice, a smaller volume would be presented by a liquid ring compared to a capillary bridge under the same circumstances. The maximum volume of a capillary bridge therefore was able to occur when the solid particles were just separated from each other. According to the contact law of capillary bridge in the numerical model, a maximum value of contact force can thus be achieved just before two particles get in contact (Figure 5.4.3.3). The contact force would then decrease to a much smaller value when the contact occurs. The reduction in force can be related to the decreased volume of a capillary bridge, which can be estimated from the overlap distance and the area of the particle-particle interface. A smaller value of maximum contact force can

be developed in this case compared to the situation where no liquid ring can be developed. Due to the reduction in volume, the development of liquid ring may also result in the smaller contact force after two particles are overlapped.

Additionally, it was interesting to note that capillary bridges with both predominantly concave and convex menisci could be found in specimens at low level of saturation degree. It is commonly assumed that the interparticle forces in unsaturated granular materials are generated mainly by the tensile water pressure acting inside the concave capillary bridge, instead of by the surface tension occurring on the air-liquid interface. The observations in this study show the possibility for the development of capillary bridges with the predominantly convex shape. These results may suggest that compressive water pressures, generating repulsive interparticle forces, could also develop in unsaturated granular materials (Figure 5.4.1.4). In these circumstances, only surface tension plays a role in bonding particles together. Therefore, the force on solid particles exerted by the air-liquid interface is responsible for bonding grains, and eventually producing the cohesive strength and stiffness of unsaturated granular materials (Gallipoli *et al.*, 2003; Lourenco *et al.*, 2011). However, the appearance of capillary bridges with the predominantly convex shape could mainly result from the fact that most area of the unsaturated specimens were above the pendular state.

5.5 Summary

To observe the spatial distribution and geometrical information of capillary bridges, a series of saturation degrees ($S_r = 6\%, 9\% \text{ and } 12\%$) were

specifically imposed to the particle assemblies consisting of spherical glass beads ($d \approx 0.05mm$). X-ray CT was then conducted. Image processing was applied to statistically analyse the three phases in unsaturated materials.

Using image thresholding, the estimated values of material properties including porosities and saturation degrees were found to be close to the target values in all specimens. Identical particle size distribution (PSD) curves also could be found in all specimens. The size distribution of liquid contacts is also plotted against the saturation degree for each specimen. Results appeared to show that capillary bridges and liquid clusters may start to emerge and develop into liquid ganglia with larger sizes when a certain limit of saturation degree was achieved ($9\% < S_{r_l} < 12\%$).

The observations in this study may also suggest that the capillary bridge, at the micrometre scale, contradicts several previous assumptions in the numerical model. A variety of meniscus shapes may be developed in an unsaturated specimen with a given saturation degree, and a certain contact angle between air-liquid interfaces and particles. The formation of a liquid ring could also be found between two contacting particles due to the particle-particle interface. The evolution of the contact force between two particles, involving the development of liquid ring, was also investigated. The results appear to imply that a reduction in the contact force may be developed when a pair of particles are in contact.

CHAPTER 6: Microscopic Investigations of Unsaturated Soil

6.1 Introduction

In DEM models, for particles with the same size, the reduced suction value could result in an increased capillary bridge volume and longer rupture distance for every single pair of particles. This would eventually lead to a higher saturation degree. In practical engineering, however the change of water content in an unsaturated soil material is not dependent on the matric suction. It may be unreasonable to assume that a certain amount of water can appear or disappear uniformly among the unsaturated soil material. The increase of saturation degree, for example caused by precipitation, may only lead to a change of suction in localized areas within the soil matrix.

According to the simulation results from different distribution models, it was found that the volume magnitude for capillary effect could be an important factor leading to the higher strength of an unsaturated material. Similar stress-strain behaviour was found among different distribution models with the same volume magnitude of capillary effect. A simplified distribution model thus might be a good representative for unsaturated material with random distribution of liquid phase. By conducting triaxial test simulations with simplified distribution models, it was found that higher strength could be produced from a medium with larger liquid volume fraction, but with lower degree of saturation. Previous simulations with uniform capillary effect indicated that for unsaturated material in the pendular regime, a higher saturation degree could lead to higher strength.

However, this might not be true in practical problems as the liquid phase is more likely to be randomly distributed. It is possible that the density of the capillary effect varies throughout the material, for example an unsaturated assembly with some dry areas, some areas in the pendular regime and some areas beyond. The X-ray images in the previous chapter also showed evidence of this phenomenon. To further understand the origin of strength caused by the appearance of the liquid phase, it is important to investigate the capillary bridge and its mechanism at a microscopic level.

This chapter will firstly provide a preliminary study of the micromechanics of unsaturated granular assemblies at critical state. Numerical specimens with uniform capillary effects were adopted, and triaxial shearing was applied to both loose and dense specimens at different stress levels with various suctions. With the implementation of different distribution models, the study of liquid distribution at particle scale will be presented later. The relationship between material strength and various microscopic parameters was investigated. The roles of water coordination number, matric suction, saturation degree, liquid volume magnitude and density distribution of capillary effects were further discussed. The influences of particle size and packing density on capillary strengthening were also presented. A cubic model was then presented to describe the liquid volume magnitude and the density distribution of capillary effects.

6.2 Micro Responses of Triaxial Loading

During the previous DEM simulations, the contact force network and fabric were also obtained as particle scale quantities. The microscopic characteristics of dry

granular materials at critical state have been examined by researchers from different aspects such as fabric anisotropy and force transmission pattern (Huang *et al.*, 2014; Guo and Zhao, 2013; Kuhn, 2016). As a good indication of stress-induced fabric evolution during triaxial loading, the degree of fabric anisotropy also could be employed to understand the transmission pattern of capillary forces. Sample specimens with uniform capillary effects were adopted in this section. Two sets of void ratios were adopted in both dry and unsaturated specimens. Triaxial compression was carried out with numerical assemblies at different stress levels with various suctions.

6.2.1 Micro Characteristics at Critical State

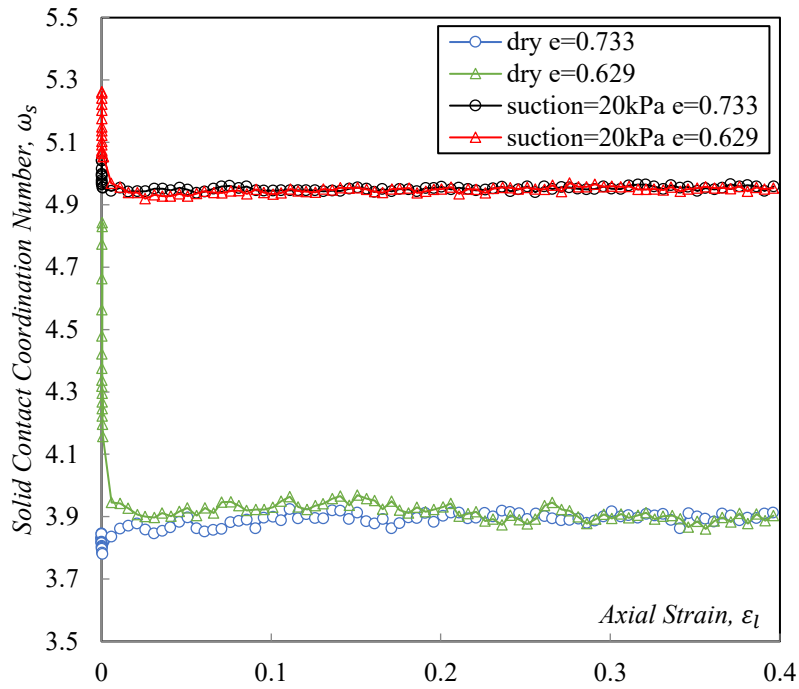
6.2.1.1 Microscopic parameters

The evolution of micro parameters under triaxial shearing is presented as an example in Figure 6.2.1.1. Both dry and wet specimens were sheared with the confining stress of 10kPa. All the wet specimens were configured with a constant suction value of 20kPa. The evolutions of both solid contact coordination numbers and water contact coordination numbers were plotted against the axial strain.

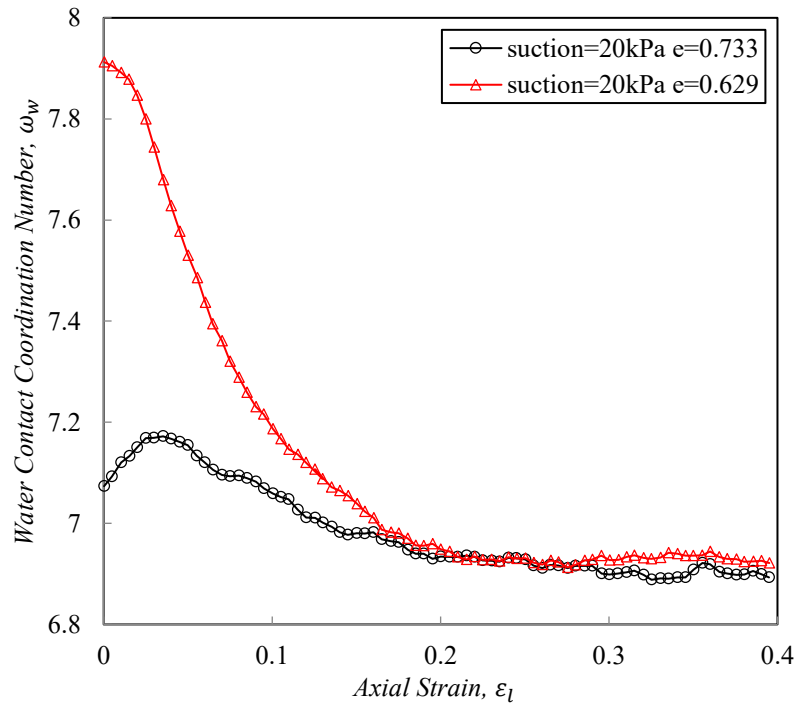
Similar to the previous results in this study, the solid contact coordination numbers observed in Figure 6.2.1.1a appear to be higher in unsaturated materials. The difference between the solid contact coordination numbers could mainly result from the attractive capillary forces. Nearly identical values of solid contact coordination number could be found at the critical states of the dry specimens,

although different values could be observed at the beginning of the compression.

Similar phenomenon could also be found with the unsaturated specimens.



(a) coordination number of solid contacts



(b) coordination number of water-solid contacts

Figure 6.2.1.1 Evolution of coordination numbers under triaxial compression simulations with uniform water distribution.

Moreover, results in Figure 6.2.1.1b appear to show that an almost identical value of water coordination number was achieved in both unsaturated materials. By comparing Figure 6.2.1.1b with Figure 6.2.1.1a, it could also be found that water contact coordination numbers were higher than solid contact coordination numbers in unsaturated materials. In the capillary bridge model applied in this study, it is assumed that bridges would form when two particles are in contact or within rupture distance. Thus, the water contact coordination numbers were always found higher than the solid contact coordination numbers in unsaturated materials.

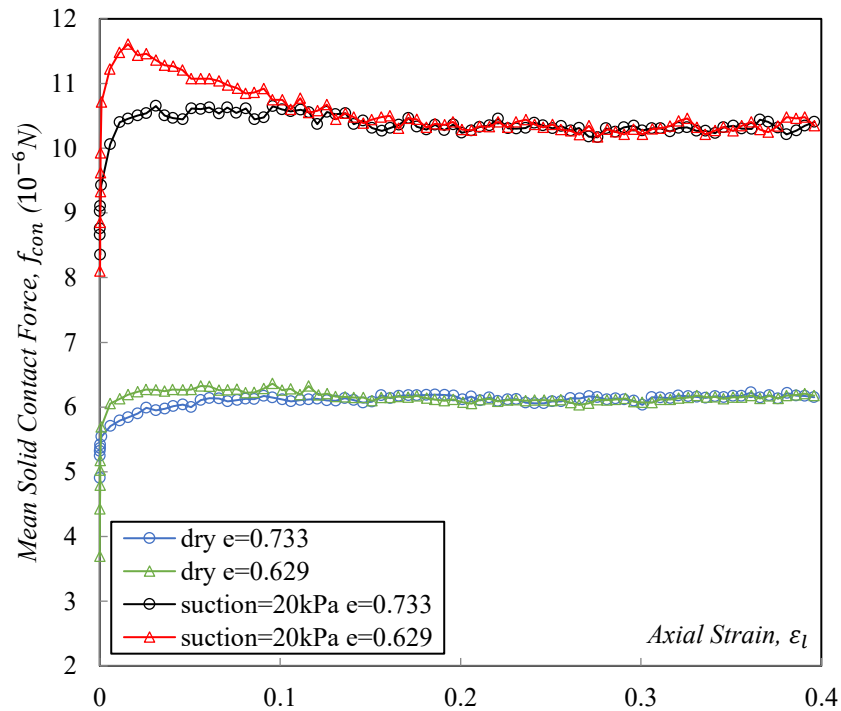


Figure 6.2.1.2 Evolution of interparticle forces under triaxial compression simulations with uniform water distribution, mean solid contact force vs. axial strain.

Similarly, the evolution of directional mean contact forces and directional mean capillary forces during the triaxial tests is plotted in Figure 6.2.1.2 and Figure 6.2.1.3. Figure 6.2.1.2 shows that the mean contact force in the unsaturated materials was larger than that in the dry specimens. The initial maximum contact

force in the dense specimens was also found to be higher than that in the loose specimens. However, after reaching the critical states, the mean contact forces were practically identical for both dry and wet specimens respectively. Moreover, Figure 6.2.1.3 indicates that a unique value for mean capillary force also could be found in both dense and loose assemblies at their critical states.

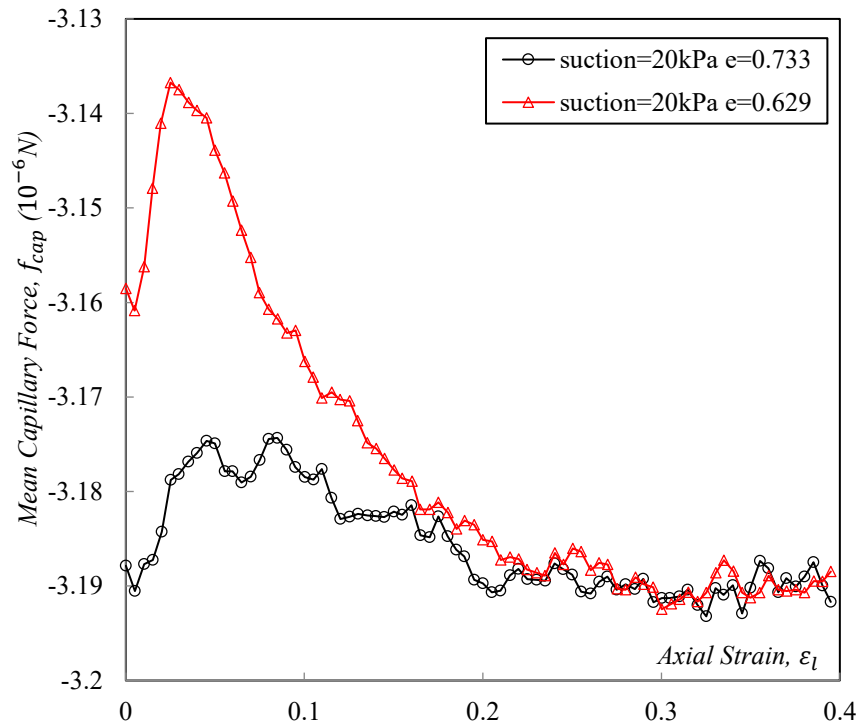


Figure 6.2.1.3 Evolution of interparticle forces under triaxial compression simulations with uniform water distribution, mean capillary force vs. axial strain.

6.2.1.2 Stress state

Figure 6.2.1.4 plots the solid contact coordination numbers in different unsaturated specimens with various suctions at critical states. For dry material, the solid contact coordination number at critical state could be found related to mean stress. Due to the higher dilatancy, solid contact coordination numbers in wet specimens at the critical state were found to be generally higher than those in dry material. When the mean stress increased, the solid contact coordination

numbers in wet granular specimens were gradually reduced. When close to the high stress level, they started to increase and approach the value of coordination number in the dry material. In Figure 6.2.1.5, it could be found that the mean contact force had a near linear relationship with mean stress level. Under low stress level, the attractive capillary effect could be found as more influential on the mean solid contact forces.

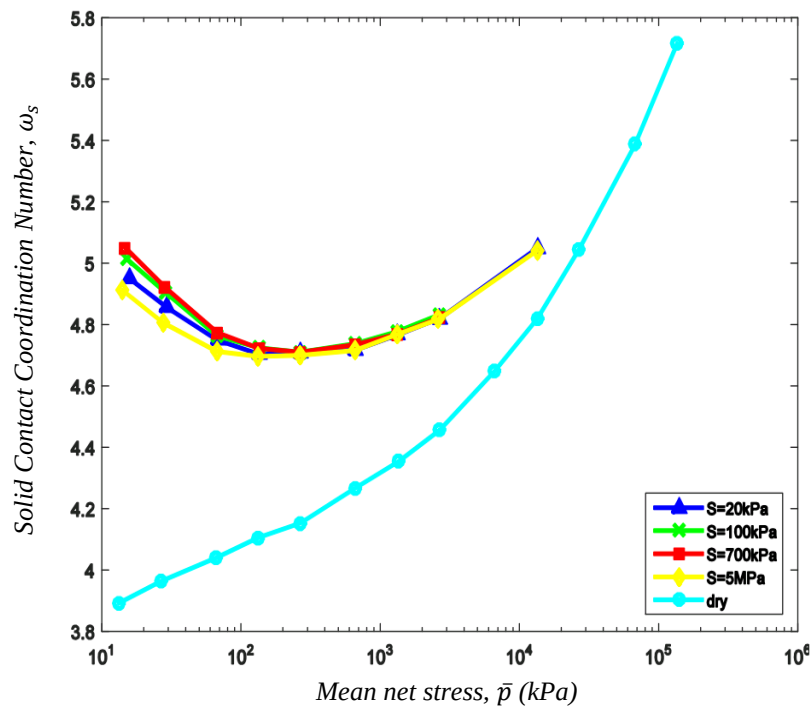


Figure 6.2.1.4 Mean contact stress vs. mean net stress, at critical state, with uniform water distribution.

As the mean capillary stress is related to the capillary bridge coordination number and mean capillary force, the values of these two factors at critical states are also presented in Figure 6.2.1.6 and Figure 6.2.1.7 respectively. It could be found that these two values were not appreciably altered by the increase of mean net stress. The mean capillary force was found as a negative value as the capillary force here acted as an attractive force. With the increase of suction (a decrease

in saturation degree), larger values of mean capillary force could be found with reduced capillary bridge coordination numbers.

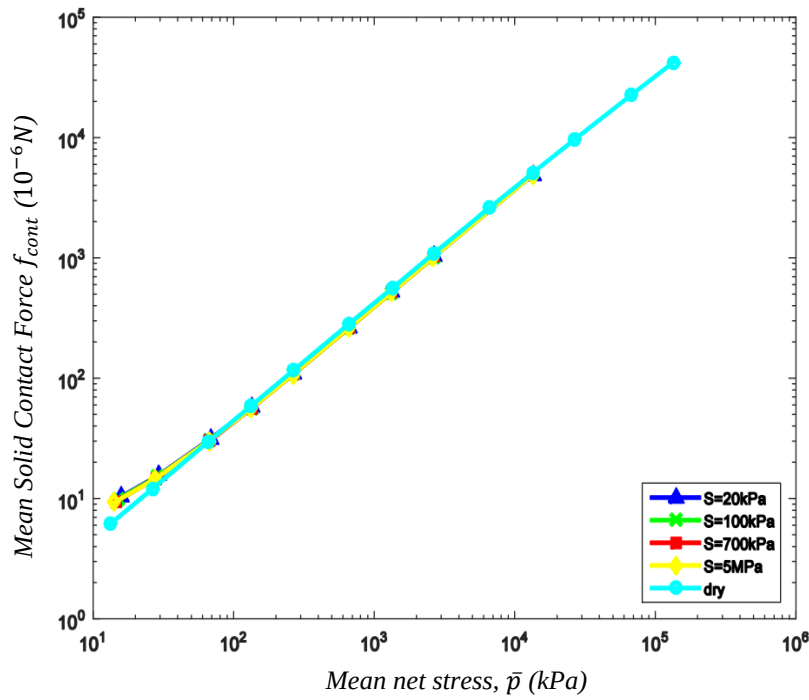


Figure 6.2.1.5 Mean solid contact force vs. mean net stress, at critical state, with uniform water distribution.

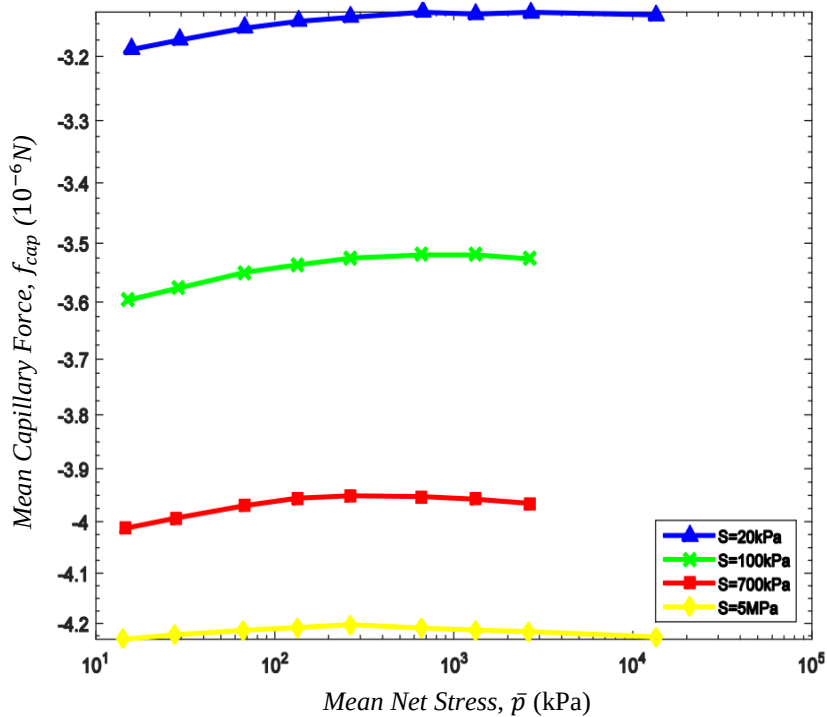


Figure 6.2.1.6 Mean capillary force vs. mean net stress, at critical state, with uniform water distribution.

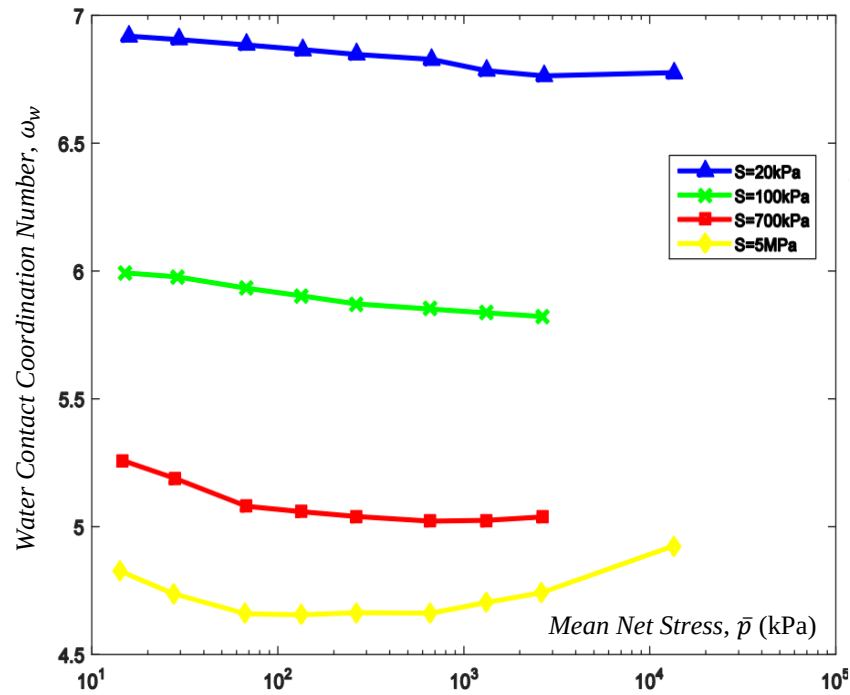


Figure 6.2.1.7 Water contact coordination number vs. mean net stress, at critical state, with uniform water distribution.

6.2.2 Uniform Distribution of Capillary Effect

6.2.2.1 Inter-particle forces

For two solid particles that are in contact, the inter-particle force is defined as the sum of the mechanical contact force and the capillary force on the capillary bridge. When the two particles are apart from each other, but within the rupture distance, the inter-particle interaction is only developed from the capillary force. The interaction between two particles vanishes when the rupture distance is exceeded. By carrying out suction controlled triaxial loading with DEM, the evolution of mean contact force with increasing stress level were plotted in Figure 6.2.2.1 (Wang, 2014). Both dry and wet specimens were employed with different packing densities ($e=0.629$, 0.688 and 0.733) and various confining stresses ($\bar{p}=20\text{kPa}$, 50kPa , 100kPa).

The largest difference between dry and wet specimens can be found from Figure 6.2.2.1, where the smallest stress level was applied. It also can be observed that the difference in mean contact force decreased when the stress level was increased. Very similar stress ratios could be found between dry and wet specimens with the same porosity when the stress level reached 100kPa (Figure 6.2.2.2). Since no capillary force was developed in the dry material, the difference in mean contact force between dry and wet specimens could be considered as representative of capillary strengthening. These results thus may indicate that the capillary strengthening effect decreased when the stress level was increased. This coincides with the macroscopic behaviour shown in chapter 4 where only a small amount of capillary strengthening could be observed after the stress level exceeded 100kPa.

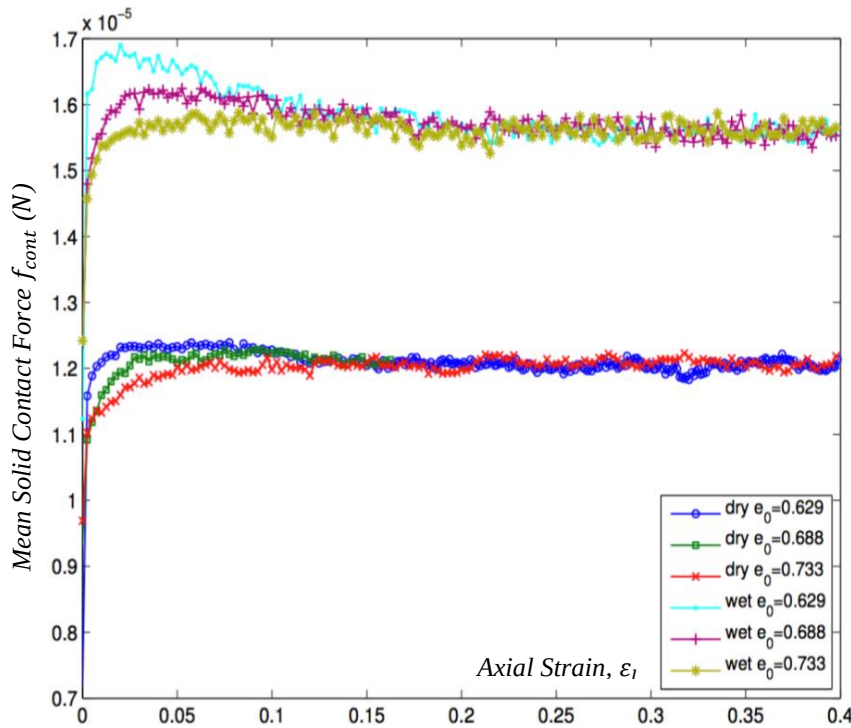


Figure 6.2.2.1 Mean solid contact force vs. axial strain, with uniform water distribution, confining stress 20kPa, suction 20kPa (Wang, 2014).

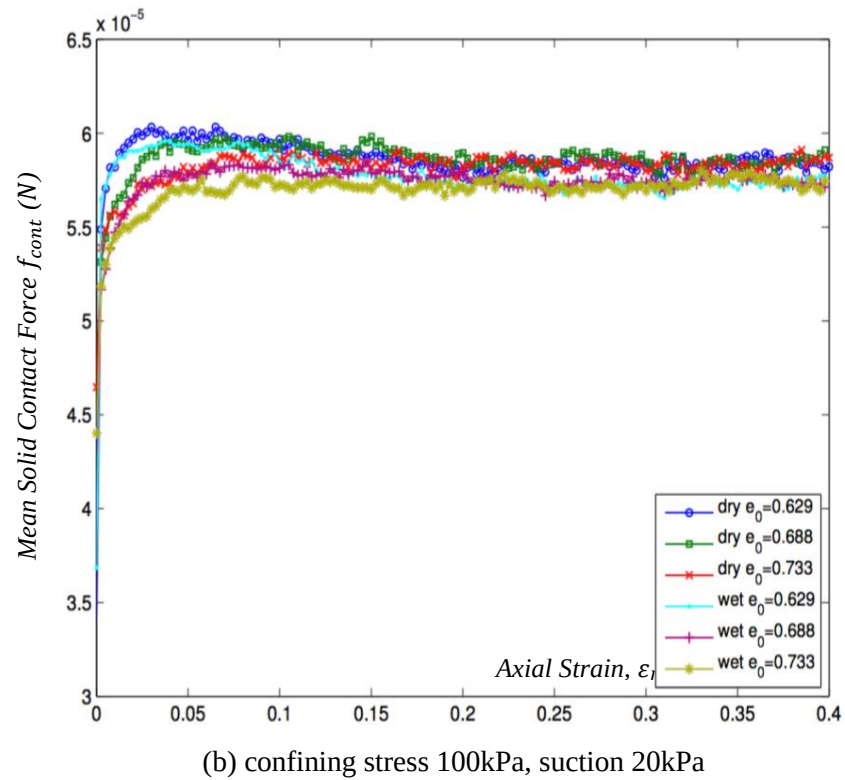
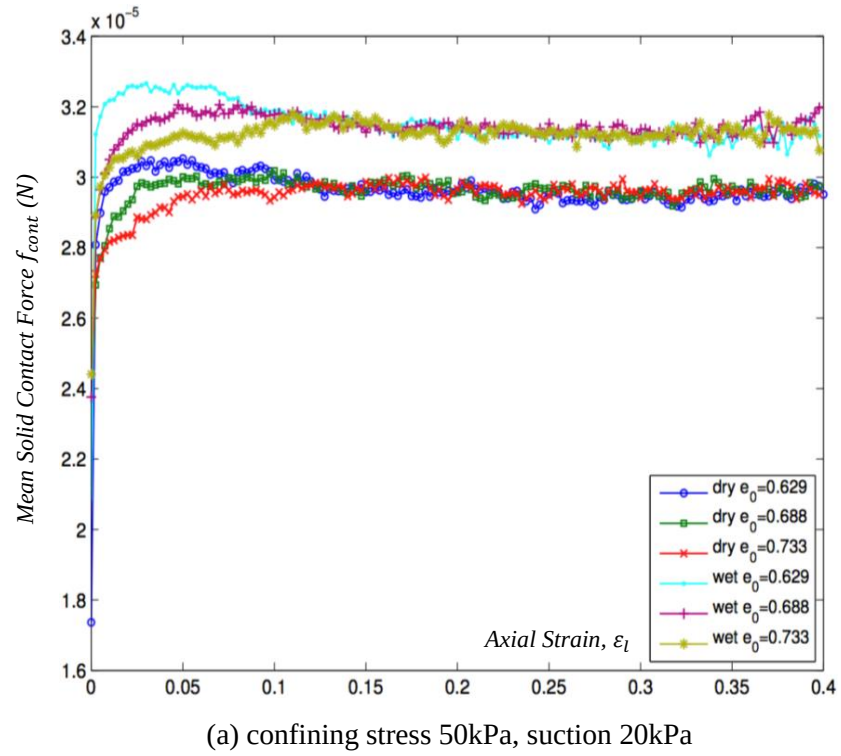
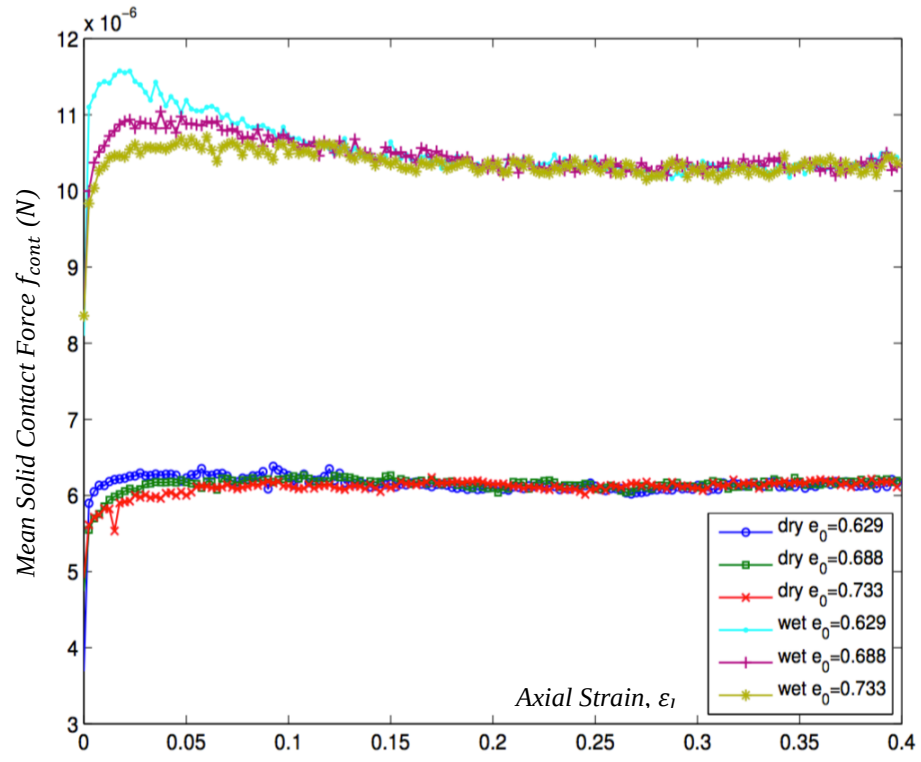


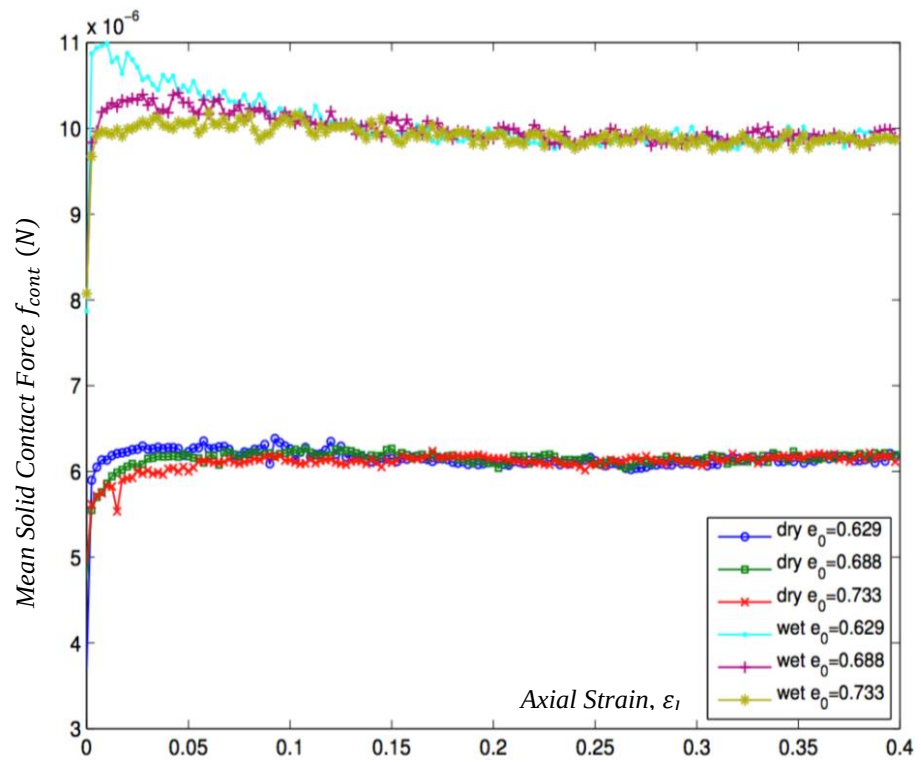
Figure 6.2.2.2 Mean solid contact force vs. axial strain, with uniform water distribution and constant suction (Wang, 2014).

Moreover, the evolution of mean contact force with increasing suction values is plotted in Figure 6.2.2.3 and Figure 6.2.2.4 (Wang, 2014). Both dry and wet assemblies were employed with different packing density and various suction values.

A small amount of increase could be found from the mean contact forces in unsaturated materials when the saturation degree was increased. The largest mean contact forces in unsaturated specimens can be found from Figure 6.2.2.3a, as the suction value here was the lowest. SWCC curves plotted in chapter 4 revealed that the saturation degree would increase while the suction value went down within the pendular regime. It also could be found that the mean contact force would decrease along with the saturation degree. This indicates that a larger mean contact force could be generated with higher saturation degree and lower matric suction, and the smallest mean contact force could occur if the residual saturation degree was achieved. Since attractive forces were generated from capillary bridges, more solid contacts also would be developed when more bridges were presented. Higher mean contact forces could result from the higher saturation degree of the material. However, without the consideration of other particle-scale parameters, such as the mean contact stress, mean capillary stress, and the coordination numbers, it is difficult to conclude that the increase in saturation degree will lead to higher strength of an unsaturated material in the pendular state.



(a) confining stress 10kPa, suction 20kPa



(b) confining stress 10kPa, suction 100kPa

Figure 6.2.2.3 Mean solid contact force vs. axial strain, with uniform water distribution and constant confining stress (Wang, 2014).

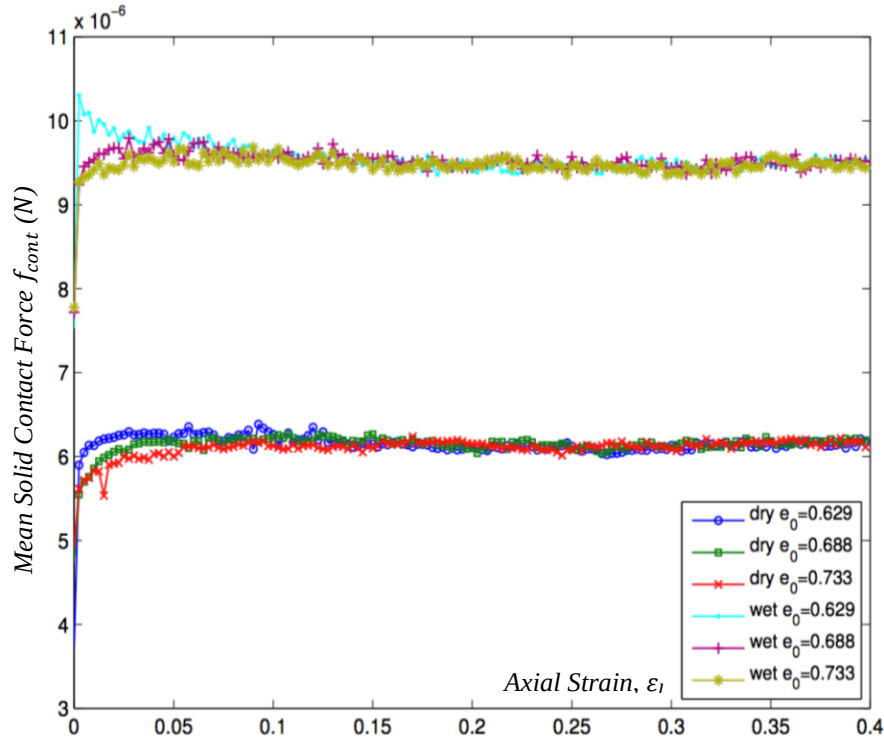
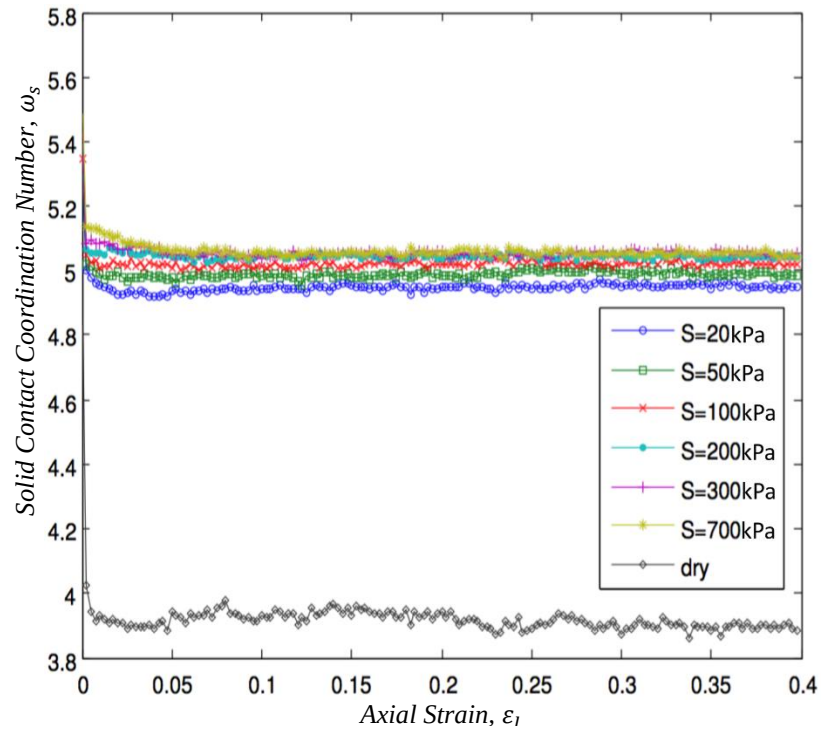


Figure 6.2.2.4 Mean solid contact force vs. axial strain, with uniform water distribution, confining stress 10kPa, suction 700kPa (Wang, 2014).

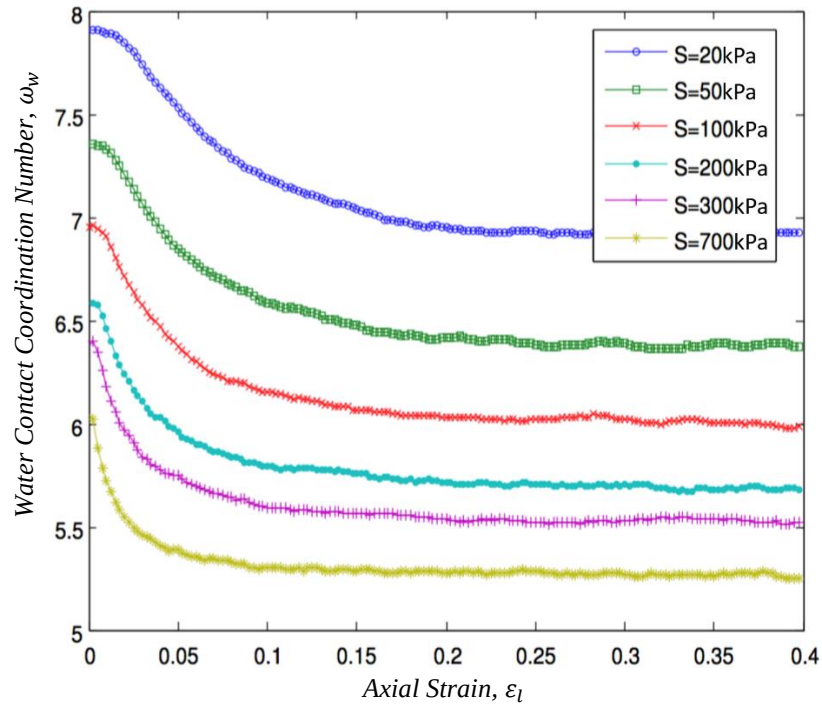
6.2.2.2 Coordination numbers

As a key factor in micromechanics of granular materials, the coordination number describes the intensity of the particle-scale interactions. For unsaturated granulates, both solid contacts and water-solid contacts were considered due to the appearance of capillary bridges. Analysing the water coordination number in an unsaturated material could help to discover the origin of capillary strength. In the study, both solid and water coordination numbers were defined as the conventional coordination number, which was the mean number of contacts per particle. In the study presented by Wang (2014), the development of solid coordination numbers (ω_s) in triaxial test simulations was plotted for both dry materials, and unsaturated specimens with uniform capillary effects (Figure

6.2.2.5a). Figure 6.2.2.5b demonstrates the evolution of water coordination number (ω_w) for the unsaturated specimens.



(a) solid contact coordination number



(b) water contact coordination number

Figure 6.2.2.5 Coordination numbers of dry material and unsaturated material (Wang, 2014).

Figure 6.2.2.5a shows a major difference in the solid coordination numbers between the wet and dry specimens. One of the important reasons can be the attractive capillary force, which leads to a denser packing and thus more solid particle contacts in the unsaturated material. It also can be found that the sample specimen with the lowest suction (20kPa) had the lowest solid coordination number among all unsaturated materials.

In Figure 6.2.2.5b, larger water coordination numbers could be found in numerical assemblies with lower suctions which could generate higher degrees of saturation. For unsaturated materials in the pendular state, the increase of water coordination number thus might be a significant factor leading to the increase of strength. Furthermore, Figure 6.2.2.5 also suggests that the solid contact coordination number does not linearly increase with the water contact coordination number. Compared to the water contact coordination numbers in unsaturated materials, only minimal differences could be observed among the solid contact coordination numbers. This might result from the particle packing density in DEM. The solid contact coordination number might vary much more notably when a wider particle size distribution curve is applied.

6.2.3 Discussion

In this section, the critical state of unsaturated granular materials was primarily investigated by conducting a series of triaxial test simulations. Capillary bridges were developed between two neighbouring particles in the pendular state. By applying materials with different packing densities and different suctions, the

critical states were reached for both macroscopic stress-strain behaviour and microscopic parameters.

The mean stress was determined using the coordination numbers and the mean force. It was observed that, at the critical state, near-identical values were achieved in both dry and wet specimens. Moreover, the mean capillary force was also found to be independent of the mean stress level at the critical state. Similar results were also discovered with capillary bridge coordination number and mean capillary force. It was also found that the solid contact coordination number and mean contact force were more significantly influenced by the capillary effect under low stress level. This coincided with the macroscopic behaviour in the previous chapter where no significant capillary effect could be observed when the stress level exceeded 100kPa. The particle packing in DEM could be one of the reasons that alleviates the capillary effect.

As higher water content was achieved when smaller suction values were adopted, larger water coordination numbers could be found in numerical assemblies with lower suctions. This could support the observation in the previous chapter that, for unsaturated specimens in the pendular state, the increase of water coordination number could be one of the significant factors leading to increasing strength. It could also explain the macroscopic results from the simplified distribution models (Figure 4.4.3.3). The enlarged volume magnitude for the capillary effect could lead to an increase in capillary bridges, and eventually an increase in the strength of material. The results however did not imply that the increase of saturation degree could directly increase the strength. This could be

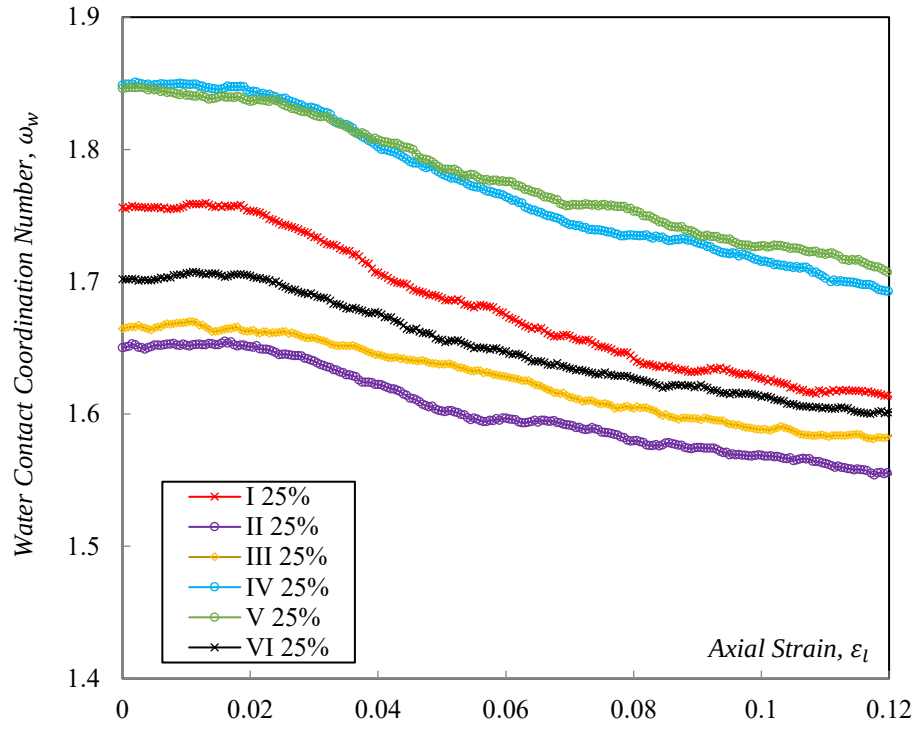
established in DEM simulations because the capillary effect was assumed to be uniformly distributed. In practical problems, the increase in saturation degree could occur at specific local areas within an unsaturated soil matrix. It is possible that less capillary bridges would be developed if the water phase was less widely distributed. To further study the origin of capillary strength, an investigation into the liquid distribution and the influence of liquid volume fraction are presented later in this chapter.

6.3 Microscopic Investigation of Liquid Distribution

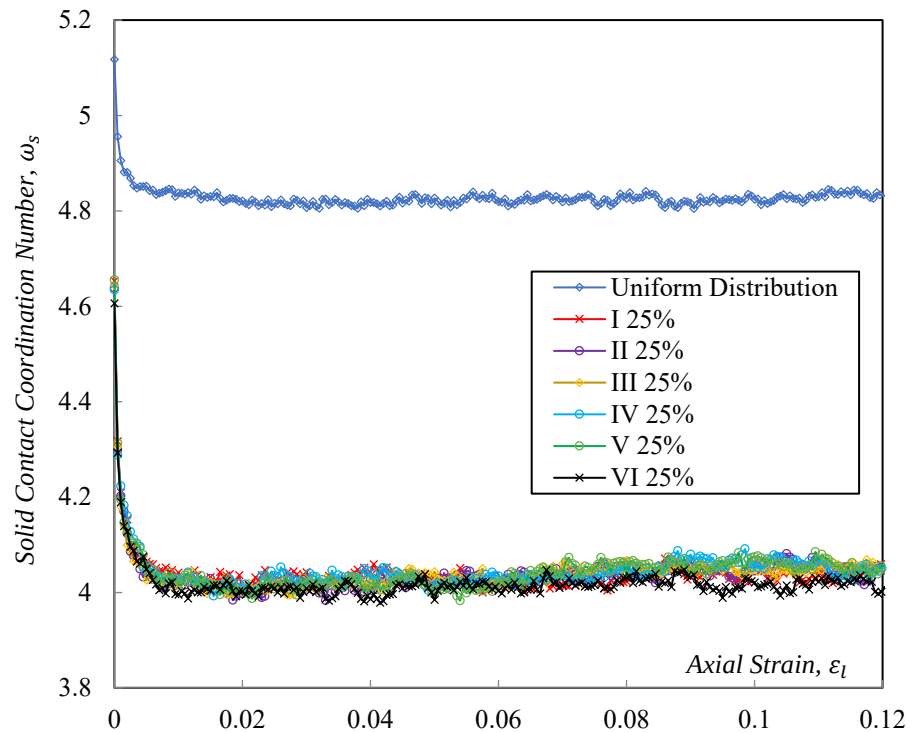
6.3.1 Micro Characteristics of Liquid Distribution

6.3.1.1 Coordination numbers

Figure 6.3.1.1a illustrates the development of water coordination number for models $I_{25\%}$ to $VI_{25\%}$ during a triaxial test simulation. It could be observed that the capillary bridge number decreased for all models when the deviatoric stress was raised. Moreover, a larger quantity of capillary bridges could be found in model $IV_{25\%}$ and $V_{25\%}$, while $II_{25\%}$ had the minimum amount of capillary bridges. As shown in the previous chapter, the liquid distribution had little influence on the macroscopic behaviour of the unsaturated assembly. This implies that for a constant soil suction, the strengthening effect of capillary bridges was not only dependent on the quantity of capillary bridges but also the geometry and the capillary force. Moreover, a much smaller number of solid contacts could be found in models $I_{25\%}$ to $VI_{25\%}$ compared to that in the unsaturated specimen with uniform water distribution (Figure 6.3.1.1b). Figure 6.3.1.2 shows that for models with larger number of capillary bridges, a larger breaking number could also be found.



(a) water contact coordination number vs. axial strain



(b) solid contact coordination number vs. axial strain

Figure 6.3.1.1 Coordination numbers of distribution models I_{25%}-VI_{25%}.

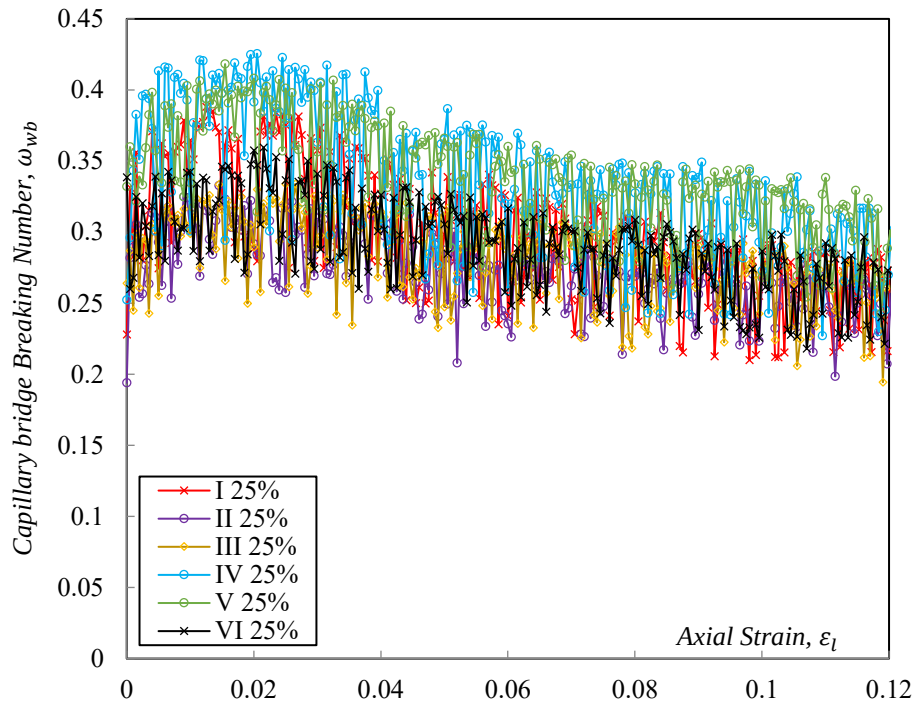


Figure 6.3.1.2 Capillary bridge breaking number of distribution models $I_{25\%}$ - $VI_{25\%}$.

Similarly, Figure 6.3.1.3 illustrates the development of these microscopic parameters for models $I_{75\%}$ to $V_{75\%}$ during triaxial test simulations. It could be observed that the water contact coordination number decreased for all distribution models when the axial strain was increased. A larger water contact coordination numbers could be found in model $III_{75\%}$ and $V_{75\%}$, while $II_{75\%}$ had the minimum values. Figure 6.3.1.4a shows the solid contact coordination number generated in models $I_{75\%}$ to $V_{75\%}$. A relatively smaller value was produced in model $II_{75\%}$, which could result from the smaller number of capillary bridges. Moreover, no significant difference could be found from the water breaking number among all models in Figure 6.3.1.4b. This was interesting to note here as less bridges were detected in model $II_{75\%}$.

By comparing the water contact coordination numbers with those from the models with smaller volume fraction of capillary effects (25%), more than three times the number of bridges could be found in models with larger volume fraction (75%). This implies the important influence of the spatial range of capillary effect distribution. In Figure 6.3.1.4a, the solid contact coordination numbers were found to be c. 4.5 per particle in models $I_{75\%}$ to $V_{75\%}$. A smaller number of c. 4 per particle was generated in models $I_{25\%}$ to $VI_{25\%}$ (Figure 6.3.1.1b). Less significant difference thus existed in the solid contact coordination number when compared to the water contact coordination number.

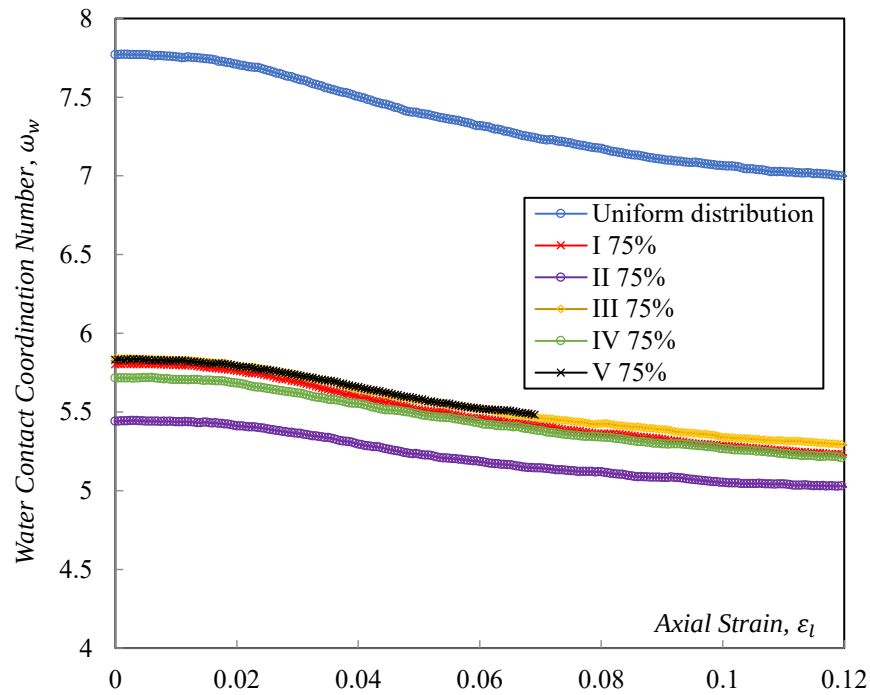
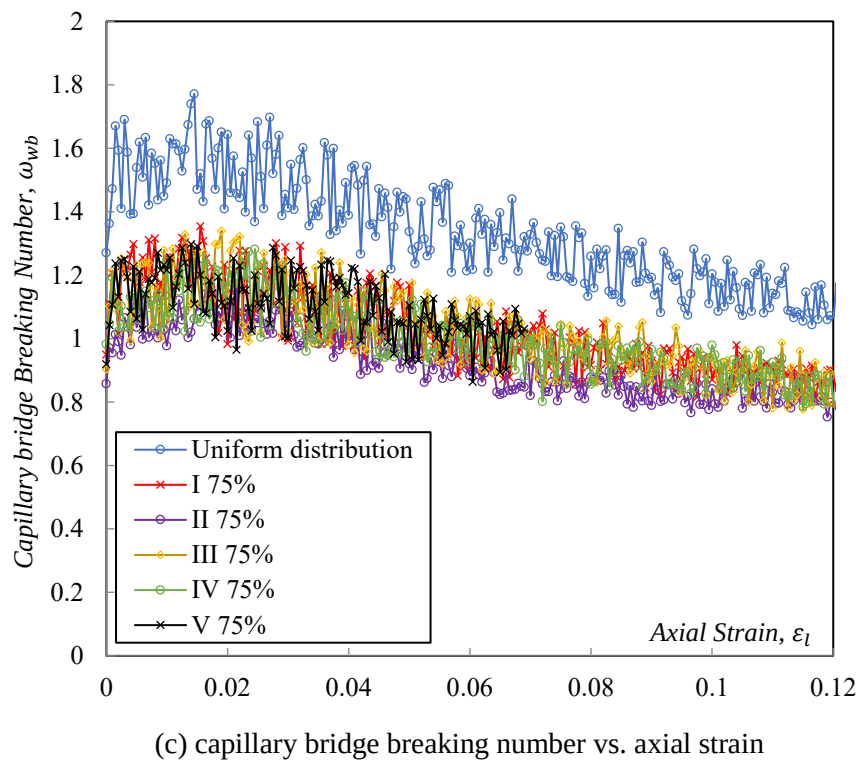
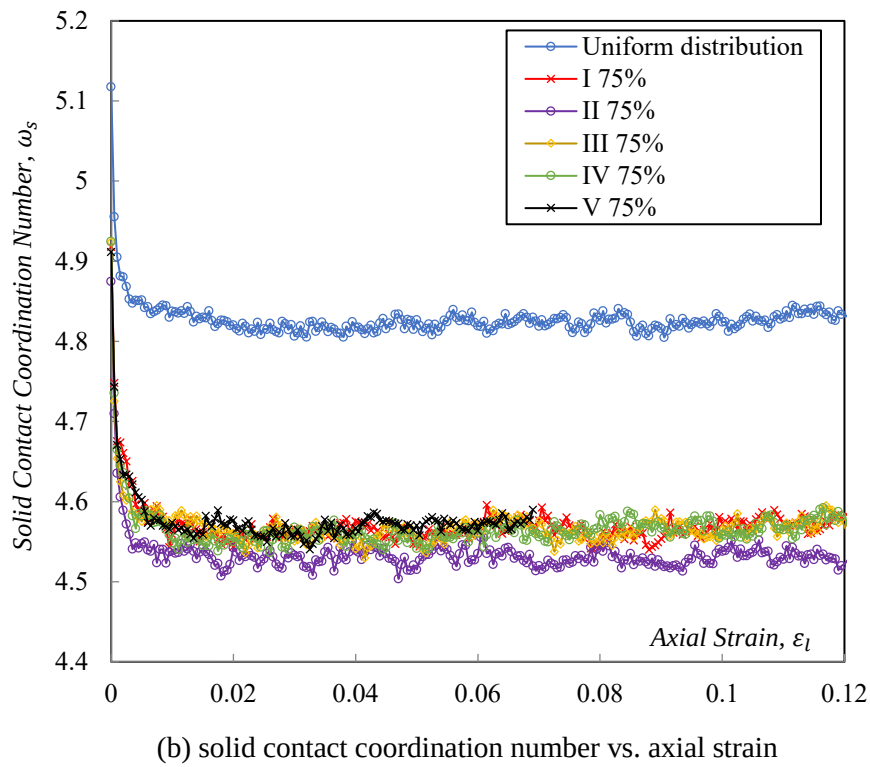


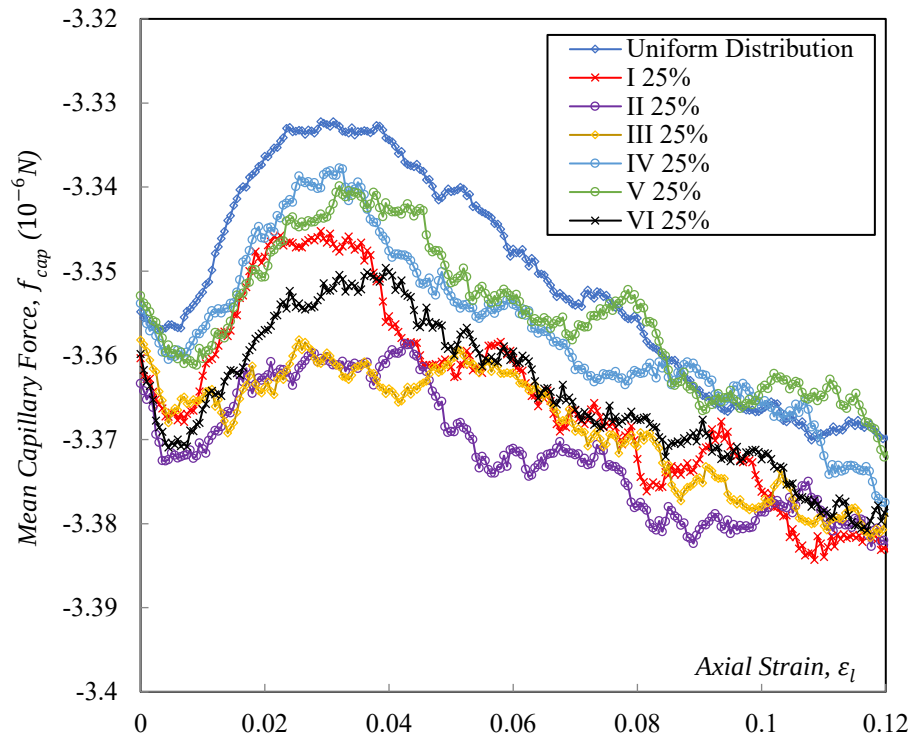
Figure 6.3.1.3 Water coordination number of distribution models $I_{75\%}$ - $V_{75\%}$.

Figure 6.3.1.4 Coordination numbers of distribution models I_{75%}-V_{75%}.

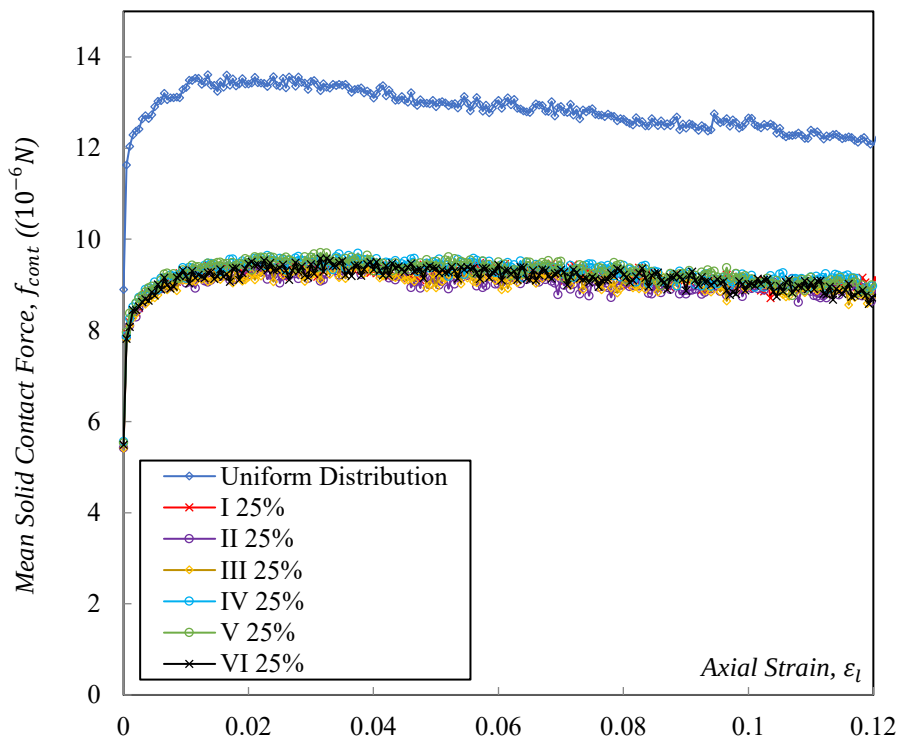
6.3.1.2 Inter-particle forces

Figure 6.3.1.5a demonstrates the changes of mean capillary forces in all distribution models $I_{25\%}$ to $VI_{25\%}$ with increasing axial strain. It could be observed that smaller capillary forces were generated from those models with a larger number of capillary bridges. The lowest values of mean capillary forces were found in the sample with uniform distribution of capillary bridges. In Figure 4.4.4 and Figure 4.4.5, results showed that a much higher stress ratio could be achieved by a numerical assembly with uniform distribution of capillary bridges, compared to specimens with localized regions of capillary effects, *i.e.* in the pendular state. This indicated that an increase in mean capillary force might not directly lead to an increasing strength of the material. Although the variance in mean capillary force was relatively small, the strength of material could be significantly increased when a larger water contact coordination number was involved.

Since the capillary bridge model in this study was established within the Young-Laplace equation, the capillary force could only be proportional to the internal radius of the capillary bridge. It could be concluded that capillary bridges with larger internal radii were generated in models $II_{25\%}$ and $III_{25\%}$, however smaller ones were produced in model $V_{25\%}$ and $VI_{25\%}$, and the smallest ones were developed in the model with uniform distribution of water. Figure 6.3.1.5b presents the evolution of mean solid contact force for models $I_{25\%}$ to $VI_{25\%}$ alongside the axial strain.



(a) mean capillary force vs. axial strain.

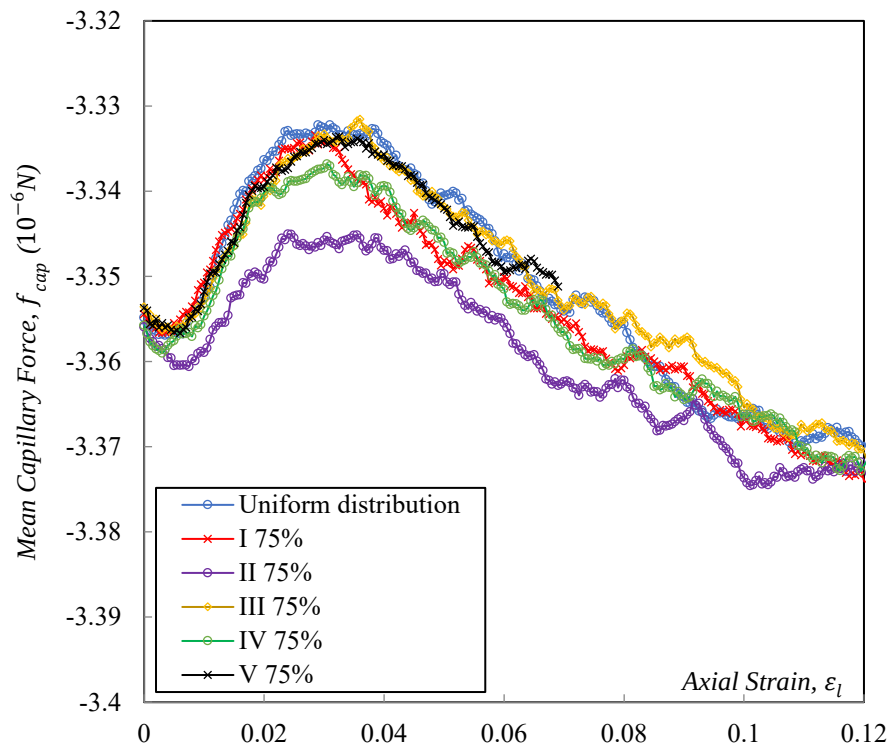


(b) mean solid contact force vs. axial strain

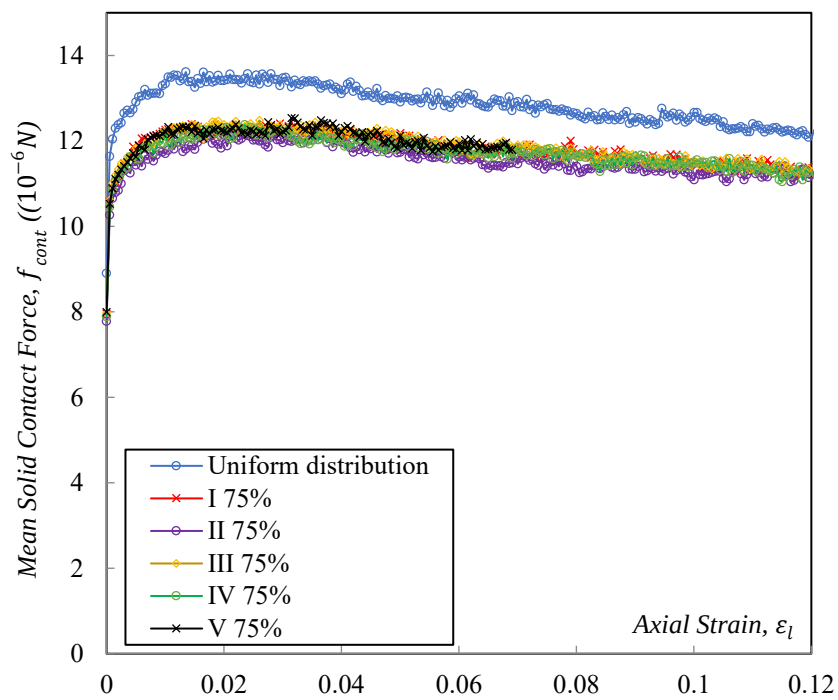
Figure 6.3.1.5 Interparticle forces of distribution models $I_{25\%}$ - $VI_{25\%}$.

Moreover, Figure 6.3.1.6a demonstrates the development of mean capillary forces in all distribution models from $I_{75\%}$ to $VI_{75\%}$. It could be concluded that almost no difference could be found when the same volume magnitude of capillary effects was used. From models $I_{75\%}$ to $VI_{75\%}$, the results all showed that smaller capillary forces were generated from those models with a larger amount of capillary bridges, and the lowest mean capillary force could be found from the assembly with uniform distribution of capillary bridges. These results match the previous results which suggested that a smaller value of suction could lead to lower mean capillary force. Figure 6.3.1.6b plots the evolution of mean contact force for all distribution models from $I_{75\%}$ to $VI_{75\%}$. These results suggest that no difference could be found when same volume magnitude of capillary effects was applied.

The results presented from Figure 6.3.1.5 to Figure 6.3.1.6 also suggested that mean capillary force increases with the volume magnitude of capillary effects. Moreover, a higher mean contact force could be found in the distribution models with larger volume magnitude of capillary effects. Among models $I_{75\%}$ to $VI_{75\%}$, larger water contact coordination numbers could be generated which caused an increase in the mean capillary force. The attractive capillary forces developed from the water-solid contact points led to an increase of solid contact coordination number which, eventually generated larger values of mean contact force.



(a) mean capillary force vs. axial strain



(b) mean solid contact force vs. axial strain.

Figure 6.3.1.6 Interparticle forces of distribution models I_{75%}-VI_{75%}.

6.3.2 Investigation with Simplified Liquid Distribution Models

By conducting the triaxial test simulations using simplified liquid distribution models which have different volume magnitudes of capillary effects ($I_{25\%}$ and $I_{75\%}$), it was found in chapter 4 that higher stress ratio could be achieved with models that had higher volume magnitude of capillary effects. Since only insignificant differences could be observed among the distribution models with the same volume magnitude of capillary effects, simplified distribution models were thus applied for further investigation. Moreover the results from the simplified distribution models implied the importance of the volume magnitude of capillary effects. It was found that the volume magnitude for capillary bridges could be a more sensitive indicator of the strength of unsaturated material in the pendular state. Previous results in this chapter proved that the water contact coordination number could be especially influential on the macroscopic strength of an unsaturated material. As a particle-scale investigation on the origin of strength, microscopic parameters such as coordination number and mean contact forces from the simplified distribution models were also obtained and studied.

6.3.2.1 Coordination number

Figure 6.3.2.1 demonstrates the evolution of both solid and water contact coordination numbers in the simplified distribution models $I_{25\%}$ and $I_{75\%}$. Results show that both water and solid contact coordination numbers in model $I_{75\%}$ was higher than those in model $I_{25\%}$. It could also be found that in the model $I_{75\%}$, the water contact coordination number is higher than the solid contact coordination number. This was found to be similar to the result obtained from the model with uniform liquid distribution. In model $I_{25\%}$, however the solid contact

coordination number could be observed to be higher compared to the water contact coordination number. The extreme low value of water contact coordination number in model $I_{25\%}$ could be the result of the low volume magnitude for capillary effects, which also caused the low value of solid contact coordination number. Both water and solid contact coordination numbers were found to be higher in model $I_{75\%}$, which eventually led to an increased strength.

Figure 6.2.2.5a suggested that the solid contact coordination numbers in unsaturated materials with uniform liquid distribution were not significantly dominated by the saturation degree. However, Figure 6.3.2.1 shows that the value is strongly influenced by the volume magnitude of capillary effects. The solid contact coordination number ratio thus might be a good indicator for the volume magnitude of capillary effects. For an unsaturated granular material, a larger ratio could be found if capillary effects were more widely distributed.

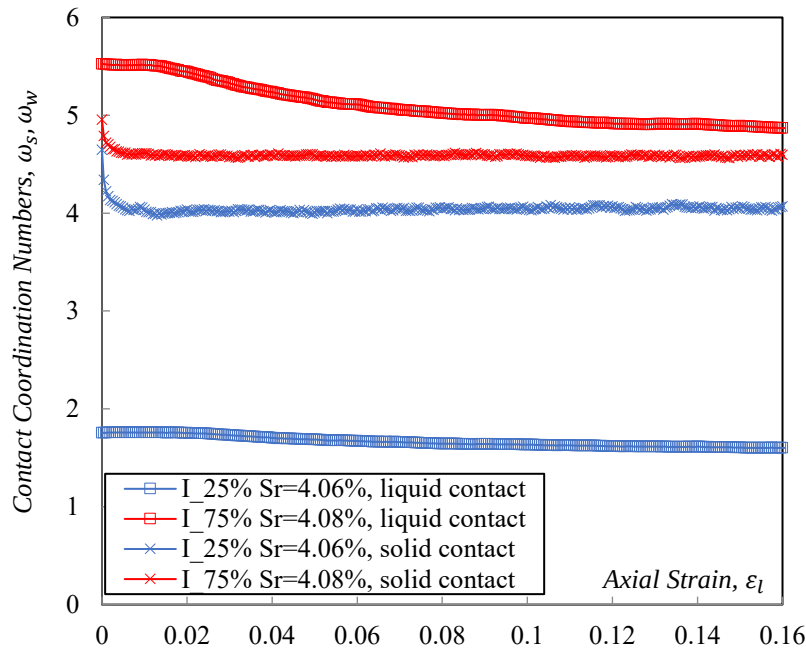


Figure 6.3.2.1 Coordination numbers of simplified distribution models ($I_{25\%}$ and $I_{75\%}$) with near-identical initial saturation degrees.

6.3.2.2 Inter-particle forces

Similarly, the evolution of mean contact forces and mean capillary forces during the triaxial tests are plotted in Figure 6.3.2.2. It could be found that neither of these two values were distinctly altered. Figure 6.3.2.2 shows that the mean contact force in model $I_{75\%}$ is larger than that in the model $I_{25\%}$. Similarly, larger mean capillary force could be also found in model $I_{75\%}$ in Figure 6.3.2.3. Larger mean capillary force is found in model $I_{75\%}$ which had a higher suction value. One of the important factors in this case could be that in model $I_{75\%}$, a higher water contact coordination number was generated. Similar results were also detected from the model with uniform water distribution. Figure 6.2.2.3 suggests that higher values of mean capillary force are produced from models with higher suction values. Low absolute values of mean capillary force thus might result from the lower suction values.

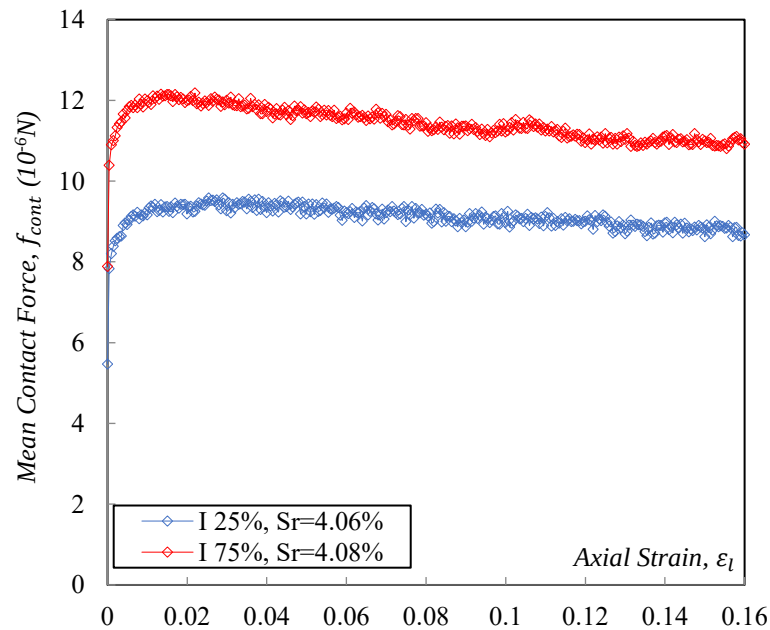


Figure 6.3.2.2 Mean contact force of simplified distribution models ($I_{25\%}$ and $I_{75\%}$).

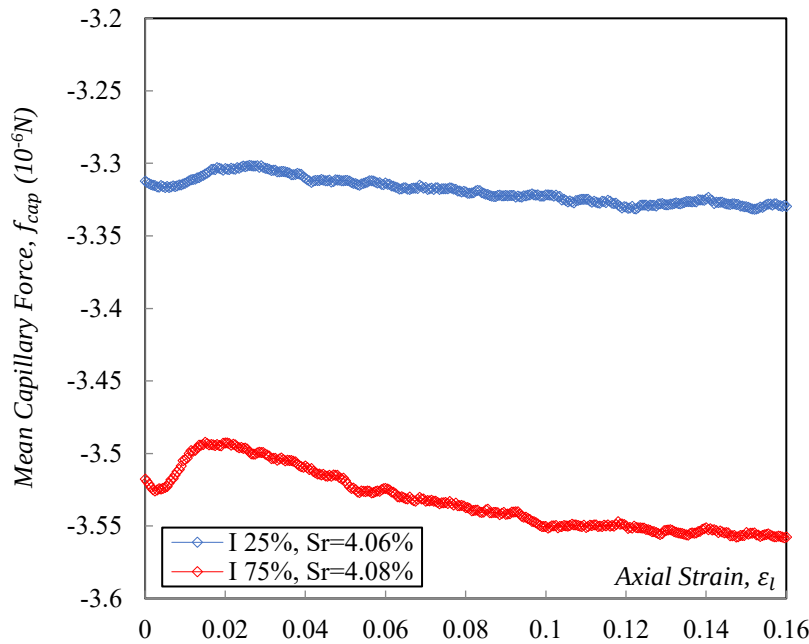


Figure 6.3.2.3 Mean capillary force of simplified distribution models ($I_{25\%}$ and $I_{75\%}$).

6.3.2.3 Investigation of particle size

The contact coordination numbers of unsaturated specimens with different particle sizes are presented in Figure 6.3.2.4 and Figure 6.3.2.5. A constant suction of 20kPa and a void ratio of 0.633 were adopted in all the specimens. Triaxial test simulations were conducted using specimens with uniform water distribution, and with random water distribution defined by model $I_{25\%}$ and $I_{75\%}$. Two values of particle radii ($r = 0.01mm$ or $r = 0.1mm$) were specifically imposed on each numerical specimen.

It could be found in Figure 6.3.2.4 that larger solid contact coordination numbers were generated by specimens with smaller particles. When the liquid volume fraction was lowered to 25%, the smallest solid contact coordination numbers could be found from specimens with different particle sizes. Note that the solid contact coordination number from model $I_{25\%}$ with smaller particles was found

to be smaller compared to the number from model $I_{75\%}$ with larger particles. Furthermore, Figure 6.3.2.5 plots the evolution of water contact coordination number for each unsaturated specimen. Very similar water coordination numbers could be achieved by specimens with the same liquid volume fraction. This implies that the differences in solid contact numbers in Figure 6.3.2.4 were mainly developed from the difference in particle size. Since larger stress ratios also could be achieved by all three specimens with smaller particles (Figure 4.4.3.4a), the origin of the increased material strength thus was related to the larger solid contact coordination number.

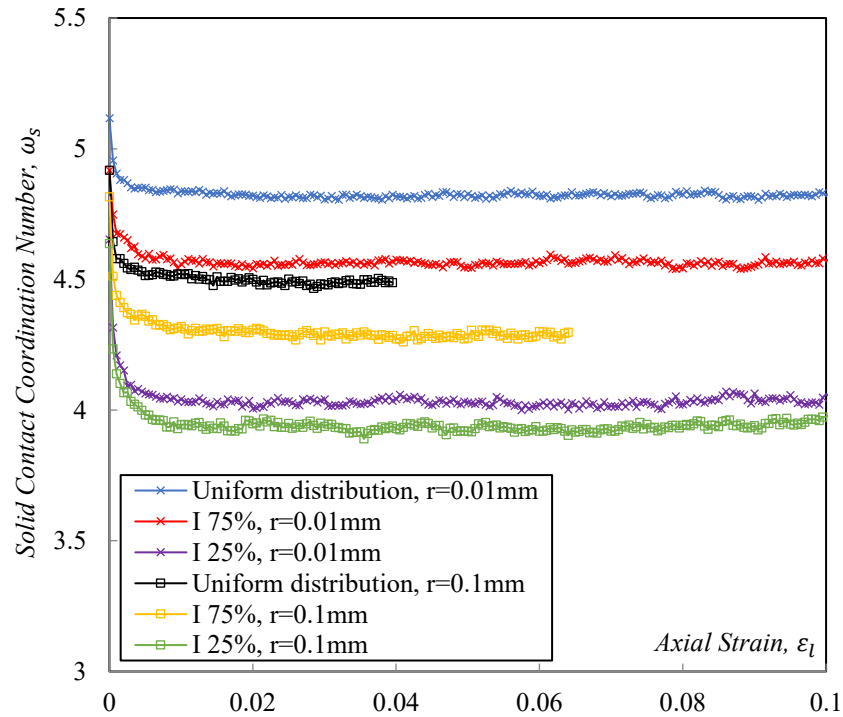


Figure 6.3.2.4 Solid contact coordination numbers of unsaturated specimens with different particle sizes.

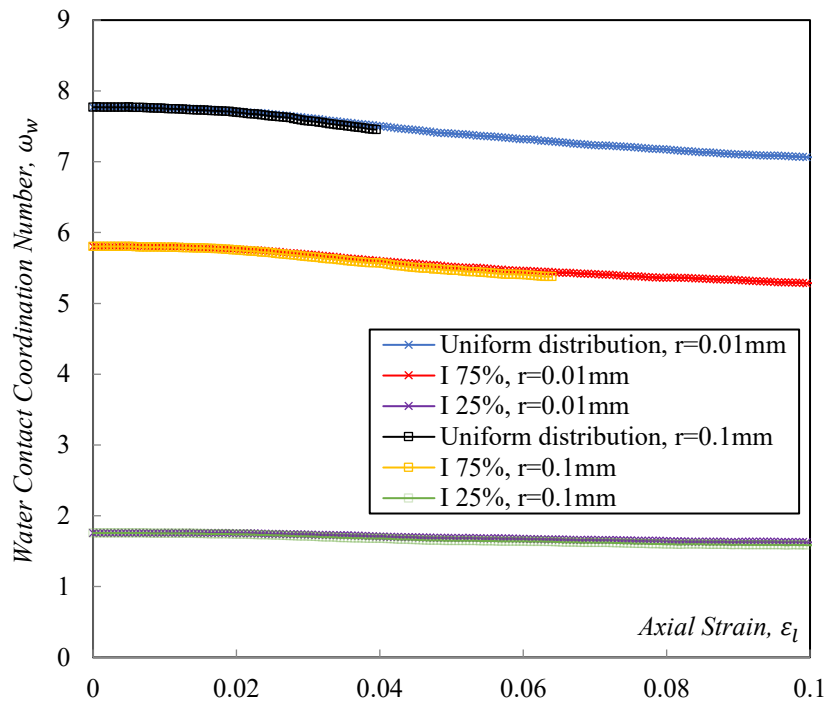


Figure 6.3.2.5 Water contact coordination numbers of unsaturated specimens with different particle sizes.

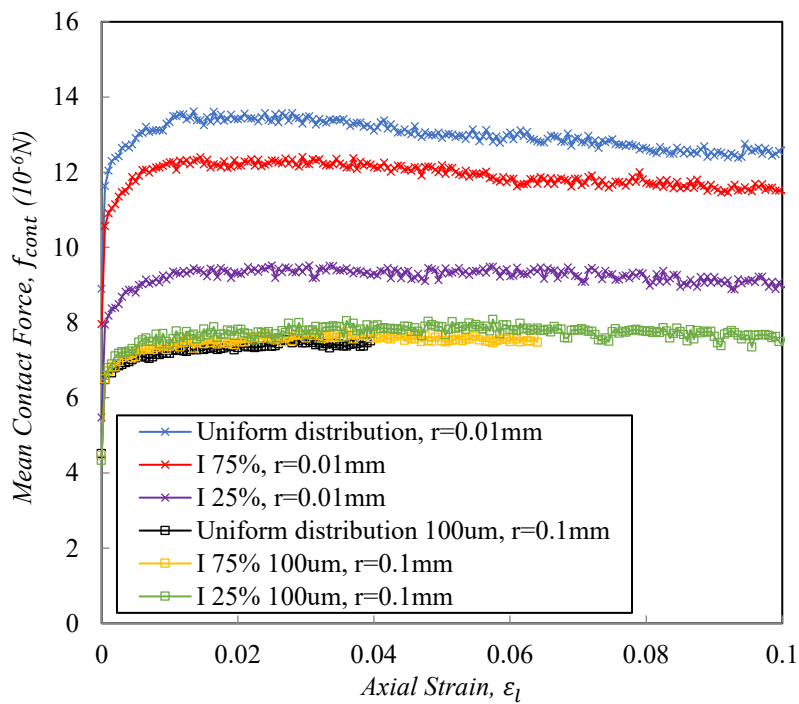


Figure 6.3.2.6 Mean contact force of unsaturated specimens with different particle sizes.

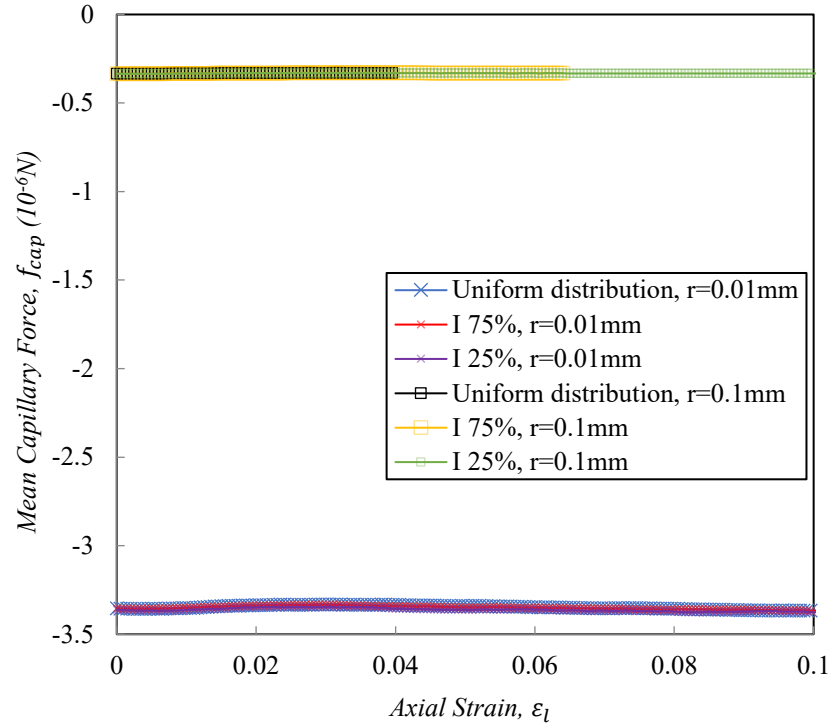


Figure 6.3.2.7 Mean capillary force of unsaturated specimens with different particle sizes.

The evolution of the interparticle force developed by each unsaturated specimen was presented in Figure 6.3.2.6 and Figure 6.3.2.7. It could be found in Figure 6.3.2.6 that significantly larger mean solid contact forces were developed by specimens with smaller particles. The larger solid contact force could result from the larger mean capillary force in Figure 6.3.2.7. For the specimens consisting of larger particles, a reduction in the solid contact forces moreover could be observed when lower liquid volume fraction was adopted. The opposite results were detected in specimens with larger particles. The largest solid contact forces were developed in model I_{25%}, whilst the smallest values could be found from the model with the uniform water distribution. Although a larger mean capillary force was developed by the specimens with smaller particles, no major difference could be found amongst the specimens with the same particle size.

Although near-identical saturation degrees and water contact coordination numbers could be found from the specimens with different particle sizes, larger interparticle forces still occurred. For unsaturated materials with different magnitudes of particle sizes, better strength can thus be achieved by these with smaller particles. A higher solid contact coordination number can be developed due to the smaller particle size involved. Larger interparticle forces can result from the smaller contacting areas.

6.3.3 Discussion

The results show that both water coordination number and solid contact coordination number could be influential on the macroscopic strength of an unsaturated granular material. Compared to the dry assemblies, a higher solid contact coordination number could be found in the unsaturated specimens. This could result from the attractive capillary forces. Both coordination numbers were also found to be highly dependent on the volume magnitude of the capillary effects. Moreover, the liquid volume fraction was also determined to be especially dominant in controlling the water contact coordination number. In an unsaturated material, higher strength appears to be generated when a wider distribution of capillary bridges is developed.

The solid contact coordination number was found to be higher, compared to the water coordination number in the simplified distribution model $I_{25\%}$. This is opposite to the results obtained in the specimen with uniform liquid distribution. Since capillary bridges were permissible to form between two contacting particles in the numerical model. For the particles under the capillary effect, this

indicates that a capillary bridge can be generated for each pair of contacting particles, which can result in the occurrence of the higher water coordination number. In this case, the value of water coordination number equals the value of solid contact coordination number plus the number of capillary bridges generated between separated particles. However, the liquid phase was less widely distributed in model I_{25%}, a smaller number capillary bridges could be developed in the controlled liquid volume. Although a higher saturation degree was produced in model I_{25%}, lower stress ratio was produced when compared to model I_{75%}. This shows that the saturation degree might be an insensitive factor when being used to understand the macroscopic strength in direct relation to the capillary effect. The higher water coordination number can be developed when the same amount of water is more widely distributed, which can also lead to the higher solid contact coordination number. Eventually, the increased contact coordination numbers could result in a higher material strength.

For unsaturated materials with uniform liquid distribution, it could be found that the solid contact coordination number was not significantly influenced by the saturation degree. However, the value was strongly dominated by the volume magnitude of capillary effects. Therefore, the solid contact coordination number may also be used to express the volume magnitude of capillary effects. For the unsaturated granular materials with the similar confining stress and saturation degree, a higher solid contact coordination number may imply that the capillary bridges are more widely distributed.

Moreover, by comparing the coordination numbers with the results from X-ray CT, it could be found that the water contact coordination number is significantly over predicted in DEM. The liquid phase would also start to form clusters when a certain volume of liquid was surrounding a solid particle. To further understand the mechanism of unsaturated granular materials, a maximum value for the water coordination number could be used as the upper limit for the pendular regime.

6.4 Investigation on the Origin of Strength

6.4.1 Introduction

Unsaturated granular material consists of three phases where the particle, liquid and air interact depending on the thermodynamic equilibrium. Figure 2.1.2.3 shows the different saturation regimes according to the water content and to the void ratio of the material ([Mitarai and Nori, 2006](#)). It can be found that only capillary bridges are developed in the pendular regime, however liquid clusters start to form in the funicular state.

The shear strength of granular material is regarded as an important factor when dealing with numerous engineering applications, such as the design of retaining walls, foundations, and pavements in practical geotechnical problems. Increased attention has been devoted to unsaturated granular materials recently. The development of analysis techniques and the study on the estimation of strength parameters have rapidly advanced and expanded. The investigation of unsaturated granular materials has been progressed to various geotechnical problems, such as seepage and slope stability ([Fredlund *et al.*, 1978](#); [Lu *et al.*, 2010](#); [Chae *et al.*, 2010](#)).

A DEM model for the analysis of wet granular soils in the pendular regime has been proposed. Capillary mechanisms are described at the contact scale based upon the capillary theory in both terms of interparticle adhesive force and water retention. Capillary bridges are assigned inside the medium with different distribution patterns. As an attempt toward the understanding of capillary induced macroscopic behaviour, the present study mainly focuses on capillary bridges as defined in the pendular regime. Therefore, the modelling is limited to low saturation degrees with only the development of capillary bridges.

6.4.2 Matric Suction

Many experimental and theoretical investigations have been carried out to determine the properties of unsaturated granular material and understand its mechanical behaviour. After Bishop's pioneering work in the 1950s, numerous studies focusing on demonstrating the relationship between matric suction and shear strength of unsaturated soil have been presented ([Bishop, 1959](#); [Fredlund *et al.*, 1978](#); [Khalili and Khabbaz, 1998](#); [Tekinsoy, *et al.*, 2004](#); [Schnellmann *et al.*, 2013](#)). Two main approaches are widely used, which are the effective stress approach and the two independent stress state variables approach. However, these solutions are limited when a wider variety of matric suction and other microscopic parameters are applied ([Vanapalli *et al.*, 1996](#); [Song *et al.*, 2011](#)).

Previous studies implied that matric suction could induce an apparent cohesion that notably increases the stability of an unsaturated granular material. The reduction of matric suction after the material is gradually saturated, significantly decreases the shear strength and stability, and ultimately may lead to failure and

collapse of an unsaturated material. However, with the development of DEM method, opposite phenomenon has been found when the material is assumed under pendular regime where only capillary bridges are developed. Large number of researches have been carried out aiming on the inter-particle capillary bridge uniformly distributed in the pendular regime (Hotta *et al.*, 1974; Lian *et al.*, 1993; Soulié *et al.*, 2006b).

The results in this study also confirm that lower matric suction can lead to the increasing strength and stability of an unsaturated granular material in the pendular regime. SWCC curves were firstly generated to analyse the relationship between saturation degree and matric suction under pendular regime. It could be observed in Figure 4.4.2.1 and Figure 4.4.2.2 that the increasing saturation degree could be related to the reduction in matric suction. According to the capillary bridge model applied in this study, Equation 3.2.28 shows that the geometry of the bridge is dependent on the constant value of matric suction. Study proposed by Wang (2014) showed that, using the toroidal approximation for capillary bridge geometries, larger volume of a single capillary bridge and longer rupture distance could be developed when the matric suction was decreased. Furthermore, it could be found in Figure 6.2.2.5b that larger water contact coordination number was related to the decreasing matric suction. It might explain that higher saturation degree can be found in the materials with lower matric suction. The results in this study may suggest that for unsaturated granular materials in the pendular regime, the reduction in matric suction can lead to the increase of both liquid volume fraction and water contact coordination number, and eventually result in a better strength and stability.

To conclude, the decreasing matric suction can firstly benefit the strength of unsaturated material in the pendular regime. This is because of the increased liquid volume fraction and the growing water contact coordination number whilst the saturation degree is raised. More capillary bridges are generated when the saturation degree is increased but limited within the pendular regime. The strength of the material then decreases gradually after the saturation degree achieves the upper limit of pendular regime, where liquid clusters start to generate from capillary bridges.

6.4.3 Degree of Saturation

In previous studies, the interparticle capillary effect has been dealt with a great attention in the pendular regime ([Hotta *et al.*, 1974](#); [Lian *et al.*, 1993](#); [Soulié, *et al.*, 2006a](#); [Soulié, *et al.*, 2006b](#)). In DEM models, for particles with same sizes, the reduced matric suction value could result in the increased capillary bridge volume and longer rupture distance for every single pair of particles. This eventually led to the higher saturation degree and larger number of water contact coordination number. However, the modelling for the distribution of liquid phase remains an ambiguity.

By increasing normal forces at the liquid-particle contacts, capillary bridges could contribute to the increasing stiffness of the material due to the appearance of cohesion. The results in this study imply that capillary-induced attractive forces and water contact coordination number play a significant role in the shear strength of unsaturated granular materials. Previous simulations with uniform capillary effect indicated that for unsaturated material in the pendular regime, a

higher saturation degree could lead to better strength. However, this might not be true in practice as the liquid phase is more likely to be randomly distributed. For example, in an unsaturated material, some areas may be at the pendular state while other areas can be dry. From the investigation on the liquid distribution, results show that the capillary bridge density is not simply dependent on the saturation degree. It is found that the strength of an assembly is mainly dependent on the capillary bridge density. By conducting the triaxial test simulations with the simplified distribution models, it was found that higher strength could be produced from the medium with larger volume magnitude of capillary effects, but with lower degree of saturation. The volume magnitude of capillary effects therefore can be another factor that can significantly impact the capillary bridge density.

It can be concluded that the increase of saturation degree may not directly link to the increase of water contact coordination number and the better strength even when the material is in the pendular regime. With the consideration of liquid distribution, DEM simulations conducted in this study show that the volume magnitude for capillary effects can be a more influential factor contributing to the strength of unsaturated granular material compared to the saturation degree. It suggests that the strength and the stability of an unsaturated material are mainly dependent on the capillary bridge density, *e.g.* the water contact coordination number per particle.

However, it may be irrational to consider a global degree of saturation in the SWRC curves in DEM, where suction is governed by the local water distribution.

To better analyse the effect of capillary bridge distribution, further study can be carried out using a local Sr-S relationship.

6.4.4 Contact Coordination Numbers

The results in this study showed that both water coordination number and solid contact coordination number could be influential on the strength and stability of an unsaturated granular material. For unsaturated materials with various degrees of saturation in the pendular regime, higher strength was presented when higher saturation degree and lower matric suction were applied. However, when implementing the simplified distribution models, increased stability was found in the specimen with lower saturation degree and higher matric suction. This is because more capillary bridges can be developed in the specimen with larger volume magnitude of capillary effects. Therefore, a larger amount of contact coordination numbers is required to generate an increased strength.

Due to the attractive capillary forces, higher solid contact coordination number can be found in unsaturated specimens compared to that in dry specimens. However, only the water contact coordination number appeared to be highly dependent on the liquid volume fraction. For unsaturated materials with uniform liquid distribution, observations also show that only minor influence could be found in the solid contact coordination number when the saturation degree was increased.

In summary, more capillary bridges may be developed when a specific amount of water is in a larger volume. Only minor difference could be observed in the

solid coordination number and the interparticle forces when the liquid volume fraction was increased. The effect of water coordination number may be considered as much more significant for an unsaturated material in the pendular regime. For unsaturated soils with the uniform water distribution and the similar particle packing, the ratio of water to solid contact coordination number may also be an effective indicator for the soil strength that is increased by the capillary effect. Higher strength in an unsaturated material could be achieved if a larger ratio of coordination number is determined.

6.5 Summary

In this chapter, the microscopic investigation was firstly carried out for the unsaturated materials at critical state, with the uniform distribution of capillary effect. The results appear to show that the capillary strengthening effect may be highly related to the development of contact coordination numbers of water and solid. Compared to the dry assembly, higher solid contact coordination number could be found in unsaturated specimens due to the development of the attractive capillary forces. For an unsaturated material with uniform water distribution, the results may also suggest that the higher strength may be developed when a larger ratio of coordination number ($\frac{\omega_w}{\omega_s}$) is determined.

For the unsaturated assembly with uneven water distribution, it was observed that both solid and water contact coordination numbers were dependent on the liquid volume fraction. Higher contact coordination numbers can be developed when the same amount of water is more widely distributed, which may also lead

to the higher material strength. Moreover, the liquid volume fraction appeared to be significantly influential in controlling the water contact coordination number.

Since only minor difference could be observed in the solid contact coordination number and the interparticle forces when the liquid volume fraction was altered, the water coordination number may be considered as a much more significant factor contributing the strength of an unsaturated material in the pendular regime. However, the overprediction in the water contact coordination number could be found in DEM when compared to the experimental observations. To better reproduce the mechanism of unsaturated granular materials in DEM, instead of using saturation degree as an indicator, a maximum value for the water contact coordination number may be adopted as the upper limit for the pendular regime.

CHAPTER 7: Conclusions and Suggestions

7.1 Conclusions

This study mainly focused on the comprehension of the mechanical behaviour of unsaturated granular materials at low water content by proposing a 3-dimensional numerical model using the discrete element method (DEM). As validation tests, the numerical predictions of triaxial shearing for dry granular materials was firstly carried out to compare against experimental data. By conducting the suction-controlled triaxial test simulations, the capillary strengthening effect can be confirmed for unsaturated granular materials under the pendular regime. To investigate the influence of liquid distribution in an unsaturated granular material, liquid volume fraction was introduced in the DEM model. Results appear to show that liquid volume fraction could be an important factor influencing the material strength. Moreover, no significant difference could be found in the mechanical behaviour among all distribution models with the same liquid volume fraction. This may imply that, for an unsaturated material with the random water distribution and a certain liquid volume fraction, the simplified distribution model may be considered as a good representative.

To validate the modelling results, experimental observations using X-ray computed tomography (XRCT) were carried out to determine the microscopic information of liquid contacts in glass beads assemblies with a series of imposed saturation degrees. By calculating the number of liquid contacts and determining their size distributions, it could be found that a significant number of capillary

bridges and liquid clusters would merge into each other and form connected liquid ganglia when the saturation degree reached a critical limit. Moreover, contradictions could be found between the analytical assumptions and the local geometries of capillary bridges obtained from XRCT. Results furthermore suggested the formation of liquid ring at the particle-particle interface. Since only capillary bridge is considered in the numerical model, the development of the liquid ring may result in the lower contact force for overlapped particles, and a lower maximum contact force.

A preliminary study of the micromechanics of unsaturated granular materials was provided in chapter 6. Uniform water distribution was firstly adopted to investigate the microscopic characteristics of the numerical assemblies at the critical state. The study of liquid distribution at particle scale was also presented. The roles of various microscopic parameters, such as water contact coordination number, matric suction, saturation degree and liquid volume fraction, on the material strength were discussed. The results appear to show that the capillary strengthening effect may be highly related to the development of contact coordination numbers of water and solid. For the unsaturated assembly with uneven water distribution, it was observed the liquid volume fraction appeared to be significantly influential in controlling the water contact coordination number. The higher contact coordination numbers can be developed when the same amount of water is more widely distributed, which may also lead to the higher material strength. Moreover, the overprediction in the water contact coordination number could also be found in DEM when compared to the experimental observations.

7.1.1 Role of Rolling Resistance

Investigations were firstly carried out to study the microscopic parameters in the dry granular assembly, including the coefficient of rolling resistance, angle of interparticle friction and normal and tangential stiffness. The results appear to show that the peak stress could be highly dependent on the rolling resistance. Triaxial shearing simulations were conducted as calibration tests to simulate the laboratory tests of Labenne sand. With the incorporation of the rolling resistance model, a good agreement for the deformation curve could be determined between the numerical model and the practical granular material (Figure 4.2.2.7 to Figure 4.2.2.10). It is also noted that the normal contact stiffness, and the ratio of shear to normal contact stiffness between contacting particles could dominate the deformation characteristics. Results may also imply that the dilatancy of a dry granular material might be dependent on the angle of interparticle friction. The Mohr-Coulomb failure envelop was plotted as a validation for the DEM method in modelling the mechanical behaviour of granular materials (Figure 4.2.2.5).

7.1.2 Capillary Strengthening Effect

For the modelling of the unsaturated material, the equations deliberating the capillary forces between spherical particles under the pendular regime were adopted within the Laplace-Young framework using a toroidal approximation of the capillary bridge geometry. After conducting a series of suction controlled triaxial test simulations, results in chapter 4 confirmed the strengthening effect of the capillary bridge in an unsaturated granular material. For a numerical assembly with uniform distribution of capillary bridges, it could be found that

the increasing total saturation degree could result in a higher material strength. A more significant strengthening effect also could be determined in the assembly consisting of particles with smaller sizes. However, decreased capillary effects could be observed when higher confining stress was involved. Results also suggested that the capillary effect significantly increased the dilatancy and led to a much higher ultimate volumetric strain in the unsaturated material.

7.1.3 Influence of Liquid Distribution

To study the influence of liquid distribution in unsaturated materials, different distribution models for capillary bridges were also presented in chapter 4. Six different distribution models were presented specifically for numerical specimens with different volume fractions (25% and 75%) that were permissible capillary bridge formation. By conducting the triaxial test simulations, higher stress ratios and smaller dilatancy moreover, could be achieved using specimens with larger liquid volume fraction (75%). However, identical stress-strain behaviour could be found from all distribution models with the same magnitude of liquid volume fraction. Similar developments of stress ratios and volumetric strains could be found in Figure 4.4.2.3 and Figure 4.4.2.5. The observations in this study suggested that the uniform distribution of the pore space was achieved in the numerical specimen after the isotropic compression tests. Simplified distribution models ($I_{25\%}$ and $I_{75\%}$) therefore could be considered as good representatives for particle assemblies with the same liquid volume fraction. By conducting the triaxial test simulations using identical saturation degrees, higher stress ratio was produced by the model with larger liquid volume fraction (75%). It proposed that better strength and smaller deformation could be generated if

liquid phase was more widely distributed in an unsaturated material. Thus, the liquid volume fraction could be another important factor dominating the strength of an unsaturated material.

7.1.4 Investigation of Liquid Phase with X-ray Computed Tomography

To study the geometry of capillary bridge and investigate the boundary of pendular regime, a series of saturation degrees (6%, 9% and 12%) were imposed with three sample specimens consisting of spherical glass beads with identical diameters. After conducting the image processing with Avizo Fire v8.1 software, three phases of the unsaturated specimens could be segmented specifically. The contacting particles were separated using the watershed algorithm. Different parameters for material properties, including the particle number, saturation degree and porosity were calculated and summarized in Table 5.3.1.1. Near-identical particle size distribution curves could be observed for each sample specimen (Figure 5.3.2.4). Capillary bridges, liquid clusters and liquid rings could be found in all specimens. The three types of liquid contacts were labelled and determined for each specimen (Table 5.3.1.1). The size distribution curves for the liquid contacts were also plotted (Figure 5.3.2.4). The results appeared to suggest that a significant number of capillary bridges and liquid clusters would merge into each other and form connected liquid ganglia when the saturation degree reaches a critical limit ($0.09 < S_r < 0.12$).

Images from X-ray CT moreover suggested that, in practice, capillary bridges with inconstant curvatures could develop between two solid particles without locating symmetrical to the axis passing through the particle centroids. It was

also noted that capillary bridges with both predominantly concave and convex menisci could be found in all three unsaturated specimens. The development of capillary bridges with predominantly convex shape may imply that compressive water pressures, generating repulsive interparticle forces, also could occur in unsaturated granular materials (Figure 5.4.1.4). However, the predominantly convex menisci could also result from the fact that the specimen might not at equilibrium during X-ray CT observation. Furthermore, liquid rings appeared to generate at particle-particle interfaces. The evolution of the contact force between two particles was then plotted with the consideration of liquid ring. Compared to the circumstance where only capillary bridge is involved, a decreased contact force appears to be generated when particles start to overlap, and a lower maximum contact force may be developed.

7.1.5 Origin of Strength Increased by Capillary Effect

By analysing the microscopic parameters of the unsaturated materials at critical state, the capillary strengthening effect was found to be highly related to the development of solid and water contact coordination numbers, mean capillary force and mean contact force levels. Results showed that both water and solid contact coordination numbers could affect the macroscopic strength of an unsaturated granular material. Compared to dry specimens, higher solid contact coordination number could be found in unsaturated specimens due to the attractive capillary forces. However, the overprediction in the water contact coordination number could also be determined in DEM when compared to the experimental observations.

Furthermore, higher solid contact coordination number could be found compared to the water contact coordination number in the simplified distribution model $I_{25\%}$. This was found to be opposite to the results from the specimens with uniform liquid distribution. Less capillary bridges could be formed in the controlled volume as water was less widely distributed in model $I_{25\%}$. More importantly, the liquid volume fraction appeared to be especially dominant in controlling the water contact coordination number. It could be concluded the higher strength may be achieved in an unsaturated material when capillary bridges are distributed in a larger volume. For the unsaturated material with uniform water distribution, the ratio of the water coordination number to the solid contact coordination number may be applied as a useful indicator for the soil strength that was increased by the capillary effect. The results also appear to show that the water contact coordination number could be strongly dominated by the liquid volume fraction when considering the liquid distribution. Only small difference could be observed for the interparticle forces and solid contact coordination number when the liquid volume fraction or the saturation degree was varied. For an unsaturated material in the pendular regime, the water coordination number may thus be considered as a more significant factor contributing to the increased strength.

7.2 Future Work Recommendations

7.2.1 Distribution of Water Phase

In this study, the magnitude of liquid volume fraction appeared to show the important influence on mechanical behaviour and properties of unsaturated granular materials. To validate that the water distribution has little influence on

the mechanical behaviour of unsaturated granular materials, experimental triaxial tests can be carried out in the future to compare simplified water distribution model with random water distribution pattern. For the implementation of water distribution in DEM, a more reliable analytical solution for water distribution pattern can be implemented based on the laboratory tests.

7.2.2 Capillary Effect

Based on the experimental observations in this study, several possible suggestions are presented for the better representation of capillary effect with DEM in the future. Analytical solution for the liquid ring, which can develop between two particles when they are in contact, can be established and adopted in numerical simulations. Moreover, the influence of particle size distribution on unsaturated granular materials can be further investigated, as the capillary effect was found to be highly dependent on the particle size. With the development of computational science, particles with wider distribution curves can be adopted in DEM.

7.2.3. Loading Method

The mechanical study in this thesis mainly focuses on the suction controlled triaxial compression of the unsaturated granular materials. Alternative loading methods can be adopted in the future to investigate other issues in practical engineering, for example, the laboratory vane test and the loading test considering the principal stress rotation.

7.2.4 Sample Preparation Method

Since water distribution is strongly dependent on the sample preparation, the water phase may be more evenly distributed if the specimen can be dried from a fully saturated state to a desired degree of saturation. The geometrical information and the spatial distribution of the capillary bridge can be investigated under multiple drying-wetting cycles.

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