

Numerical Evaluation of Internal Erosion due to Seepage Flow

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2017

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A thesis submitted to Imperial College London in partial fulfilment of the requirements
for the degree of Master of Philosophy in the Faculty of Engineering

Abstract

Internal erosion poses a significant threat to the stability of earth and rock-fill dams. Suffusion is one mechanism of internal erosion. Gap-graded, cohesionless and underfilled soils are susceptible to suffusion as the fine particles in this type of material are under relatively low stress. Previous research such as Skempton & Brogan (1994) has revealed that fine particles within this kind of soil are washed out due to seepage flow at much lower hydraulic gradient than critical hydraulic gradient calculated from Terzaghi's classic theory for heave, and they defined a stress reduction factor α to quantify this phenomenon. This contribution develops these concepts by using particle-scale simulation.

Hitherto, there has been a lot of attention paid to the material susceptibility, which is assessed by considering the material's particle size distribution. However, there has been little research considering the hydro-mechanical aspects of susceptibility. The hydro-mechanical aspects of susceptibility are intimately related to the particle-fluid interaction. The contribution of this thesis is to fill the gap in understanding by using the coupled discrete element method (DEM) with computational fluid dynamics (CFD) to observe the fundamental mechanisms that govern the onset of suffusion.

In this research, virtual permeameter tests with a constant head were simulated with a coupled DEM-CFD code. The permeameter simulations were validated using the work of Suzuki et al. (2007) and were compared with the results obtained from Shire (2014). Four gap-graded soils with two fines contents and two densities were investigated to consider the influence of coordination number, seepage velocity and normalised particle stress on particle displacement under varying hydraulic gradients.

Declaration

The work presented in this thesis was carried out in the Geotechnics section of the Department of Civil and Environmental Engineering at Imperial College London.

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Kenichi Kawano

11th April 2017

Acknowledgements

I would like to sincerely thank my supervisors, Dr. Catherine O’Sullivan and Dr. Thomas Shire for their support throughout my research for two years. I am deeply impressed by their passion for education and insightful feedback on my research.

This research has been funded by Kajima Corporation in Japan. Without their fully financial support, I could not have achieved my goal. I would also like to express my thanks to Mr. Jason Furtney from Itasca Consulting Group for sparing the time to sort out problems linked to the coupled PFC3D-CCFD code.

I am deeply grateful to the members in the Geotechnics section at Imperial College. Their smart ideas have cultivated profound knowledge. In particular, I would like to thank Dr. Kevin Hanley, Mr. Masahide Otsubo and Mr. Christopher Knight for their advice on the LAMMPS code and productive discussions on discrete element method and computational fluid dynamics.

My understanding has been often inspired by fruitful advice from Prof. Jonathan Fannin and his PhD students at the University of British Columbia, and Mr. Rodney Bridle at Dam Safety Ltd.

Finally, I would like to thank my parents for their support and my wife Hiroko for her encouragement during the past two years. My gratitude is also expressed to my daughter Miwa for sharing in the good times together.

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List of Notation

Symbol	Meaning
a	Magnitude of fabric anisotropy
A	Cross sectional area of soil
C	Courant number
C_D	Drag coefficient for a single spherical particle
C_{particle}	Connectivity
C_v	Coefficient of consolidation
d	Particle diameter
d_{cap}	Distance between centres of two spheres
d_{particle}	Particle displacement
D_{50}	Median diameter
D_{max}	Maximum diameter
D_{measure}	Diameter of measurement sphere
E	Void ratio
f_i	Force per particle
f_j^c	Contact force transmitted at contact position x_i^c
F	Total force
F_{drag}	Drag force per unit volume
F_{fluid}	Particle-fluid interaction force per unit volume
g	Acceleration due to gravity
h	Height of spherical cap
Δh	Head difference
H	Thickness of soil layer
i	Hydraulic gradient
i_{crit}	Critical hydraulic gradient
k	Coefficient of permeability
k_n	Spring constant (contact normal direction)
k_a	Permeability of layer a
$k_{v,\text{eff}}$	Effective permeability
L_a	Depth of soil in layer a
L	Total depth of soil
Δl	One fluid cell length
m	Particle mass

m_v	Coefficient of volume compressibility
n	Porosity
n_c	Number of particles in fluid cells
N_c	Total number of contacts
$N_{c,p}$	Number of contacts on particle p
n_i^k, n_j^k	k th unit orientation vector
N_p	Number of particles
N_p^0	Number of particles with zero contact
N_p^1	Number of particles with one contact
$N_{p,\text{fine}}$	Number of fine particles
ΔP	Fluid pressure difference
P	Fluid pressure
$\overline{P}$	Mean normal stress for entire sample
p'	Mean effective stress
$\Delta p'$	Mean effective stress increment
Q	Fluid flow
r, R	Particle radius
Re	Reynolds number
S_t	Swelling of the top surface
t	Time
Δt_e	Time step for data exchange
Δt_f	Time step for fluid
Δt_p	Time step for particle
Δt_e	Time step for data exchange
$t_{\text{simulation}}$	Simulation time step
T_v	Dimensionless time factor
u_e	Excess pore water pressure
$v_{\text{discharge}}$	Discharge velocity
v_f	Fluid velocity
v_p	Particle velocity
v_r	Relative velocity between fluid and particles
v_{seepage}	Seepage velocity
v_z	Vertical velocity of falling particle
V	Total volume (particles + voids)
V_{cap}	Volume of spherical cap
$V_{\text{intersection}}$	Volume of sphere-sphere intersection

V_p	Volume of a particle
ΔV_c	Volume of fluid cells
x	Voidage function
x_i^c	Contact position
x_i^p	Centroidal position
Δx	Difference between initial and final position in the x direction
Δy	Difference between initial and final position in the y direction
Z	Coordination number
$Z_{\text{meas,sphere}}$	Mechanical coordination number in a measurement sphere
Z_{mech}	Mechanical coordination number
Δz	Difference between initial and final position in the z direction
α	Stress reduction factor
α, p'	Average stress reduction factor (α calculated from mean normal stress)
α, σ_x	α relating to x direction
α, σ_y	α relating to y direction
α, σ_z	α relating to z direction
α_{particle}	Normalised particle stress
β	Safety factor
δ	Amount of settlement
Φ_{ij}	Fabric tensor
μ	Coefficient of friction
μ_f	Fluid viscosity
ε	Strain
θ_a	Direction of the fabric anisotropy or principal fabric
ρ_f	Fluid density
ρ_p	Particle density
ρ_{sat}	Submerged density
ρ_w	Fluid density
$\overline{\sigma_{fine}}$	Mean normal stress acting in the finer particles
$\overline{\sigma_{ij}}$	Stress acting throughout volume
$\overline{\sigma_{ij}^p}$	Average stress in particle p
$\overline{\sigma_{particle}}$	Mean normal stress for each particle
$\bar{\sigma}'_{v0}$	Vertical effective stress

Chapter 1. INTRODUCTION

1.1. Background

Earth and rock-fill dams are built for the purpose of water supply, hydraulic power generation and flood control. They are one of the most important elements of infrastructure in the world. In the UK, there are roughly 2,500 embankment dams (BRE, 1994) and 7,500 km of flood embankments (Morris et al., 2007).

It is important that embankment dams have effective filters, usually composed of granular sand and gravel, to prevent the internal erosion of the low permeability clay core due to water seepage. Internal erosion is defined as the downstream movement of soil particles from within an embankment dam by seepage flow and is probably the greatest and the least well understood hazard posed to embankment dams (Charles & Boden, 1985).

Recognising the importance of this issue, the International Commission on Large Dams (ICOLD) has set up a European Working Group (EWG) on Internal Erosion. The EWG identified three factors that contribute to internal erosion: (i) hydraulic susceptibility (ii) material (geometric) susceptibility (Shire, 2014) and (iii) mechanical susceptibility (Brown & Bridle, 2009), as shown in Venn diagram form in Figure 1.1. While macro-scale observations of the system response in laboratory tests are useful (e.g. Skempton & Brogan, 1994 and Moffat & Fannin, 2011), a complete understanding of internal erosion requires fundamental numerical investigations.

There are a wide variety of forms of internal erosion: backward erosion, concentrated leaks, contact erosion and internal instability. In this research, internal instability is the main focus. It is defined as susceptibility to the loss of fine particles in materials with distinct coarse and fine fractions. In particular, a key aspect of internal instability will be studied, i.e. the hydro-mechanical condition. The ideas that fine particles are under relatively low stress and therefore can be transported under low hydraulic gradients is central to the hydro-mechanical criterion.

Fannin et al. (2014) describe two distinct forms of internal instability: suffusion and suffosion (Figure 1.2). Suffusion is used to describe a scenario where the finer particles in the voids between the coarse fraction are washed out without any change in total volume, whereas suffosion is accompanied by the collapse of soil skeleton due to the transport of fine particles. Shire et al. (2014) suggested that the form of internal instability is related to the fines content and the density

of the soil. Internal instability can initiate at hydraulic gradients which are lower than those are expected for fluidisation or base heave (Figure 1.2 (c)) due to lower stress in the finer fraction. Current internal stability design guidelines for filters compare characteristic diameters of the coarse and fine particle fraction to determine whether the fine particles can pass through the voids between coarse particles. Specifically, they use particle size distribution (PSD)-based empirical relationships which are not completely effective (Li & Fannin, 2008). Therefore, researchers including Indraratna et al. (2007) have highlighted the need to explicitly consider constrictions between coarse particles, i.e. the geometric condition (Shire, 2014). The constriction sizes form part of the material susceptibility. While many researchers have examined the issue of material susceptibility, less attention has been paid to the hydro-mechanical aspects of susceptibility. This contribution contributes to fill the resultant gap in understanding. The fundamental mechanisms operate at the particle scale, and so the study uses particulate discrete element modelling for the particle phase coupled with computational fluid mechanics for the fluid phase.

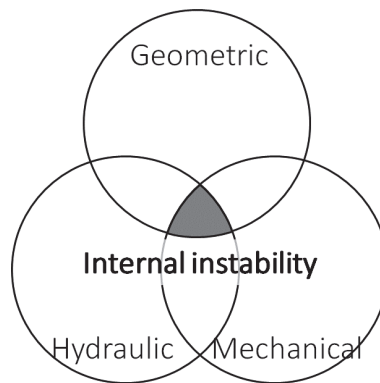


Figure 1.1 Venn diagram showing contributing to susceptibility to internal instability factors (after Garner & Fannin, 2010 and Shire, 2014)

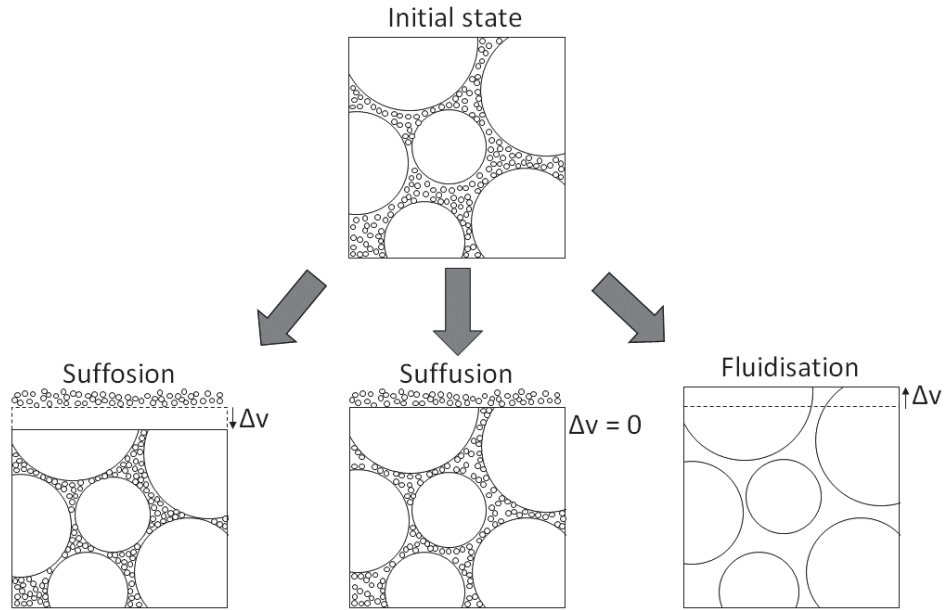


Figure 1.2 Schematic illustration of seepage-induced instability phenomena: (a) suffosion; (b) suffusion; (c) fluidisation (after Fannin et al., 2014)

1.2. Research objectives

This thesis considers suffusion or internal instability, and it is divided into three main parts: model development in Chapter 3, particle-fluid interaction in Chapter 4 and main simulations in Chapter 5.

The objectives of this contribution are to:

- Develop a procedure to simulate a constant head permeameter test using DEM coupled with CFD.
- Simulate permeameter tests on gap-graded materials with differing degrees of stress inhomogeneity, i.e. the proportion of stress carried by the finer fraction should be different.
- Analyse the particle-scale simulation data to identify characteristics associated with particles that move and interpret the results in the context of prior research: most notably, the earlier contributions of Skempton & Brogan (1994) and Shire (2014).

1.3. Outline of thesis

This thesis is organised into six chapters. In Chapter 2, the definition of key terminology related to internal instability is introduced, and a review of the relevant literature is presented. Chapter 3 explains the simulation approach considering prototype models. Chapter 4 focusses on coupled DEM-CFD simulation, where DEM is the discrete element method, and CFD is

computational fluid dynamics. Chapter 5 extends the preliminary work implemented in Chapter 3 and Chapter 4 to large samples to address the research questions presented in Section 1.2 above. Finally, conclusions resulting from this study and suggestions for future work are described in Chapter 6.

Chapter 2. LITERATURE REVIEW

This chapter discusses relevant prior research focussing on the initiation of internal instability. Section 2.1 gives a general introduction to internal erosion, focussing on suffusion or internal instability. Section 2.2 gives an overview of recent experimental research. Three main issues are considered: the impact of fluid flow on initiation of instability (Section 2.2.1), the influence of overall stress state on initiation of instability (Section 2.2.2), and the influence of stress inhomogeneity on initiation of instability (Section 2.2.3). Section 2.3 considers numerical modelling of internal instability, focussing on DEM-related research. Section 2.3.1 considers coupled simulations of internal erosion and filtration. Section 2.3.2 considers DEM studies of stress heterogeneity. Conclusions are given in Section 2.4.

2.1. Process of internal erosion

2.1.1. General introduction

From the perspective of CIRIA et al. (2013), the process of internal erosion can be divided into four stages: (i) the initiation of erosion, (ii) the continuation of erosion, (iii) the progression to form or sustain a pipe and/or to increase seepage and pore pressures in the downstream part of the embankment or its foundation, and (iv) the breach resulting in uncontrolled release of the water. In this research, the focus is on the onset of internal erosion.

Internal erosion is defined as the downstream movement of soil particles from within an embankment dam by seepage flow (ICOLD, 2015) and it has been responsible for 46% of dam failures globally (Foster et al., 2000). There are four general mechanisms causing internal erosion according to ICOLD (2015): concentrated leaks, backward erosion, contact erosion and internal instability. The aim of this study is to analyse the interaction between particles and water in internally unstable soils. In particular, internal instability is considered as this phenomenon can cause a serious damage to soil structures. For example, a sinkhole was found at the dam crest of WAC Bennett Dam in Canada as shown in Figure 2.1, resulting in a significant reduction in the supply of electricity to the British Columbia area for a few months. The term suffusion is often associated with internal instability (Fannin et al., 2014). As conceptually discussed by Garner & Fannin (2010) and illustrated in Figure 1.1, susceptibility to internal erosion depends on interlinked hydraulic, mechanical and geometric factors. The hydraulic load, i.e. seepage velocity or hydraulic gradient, must be sufficiently high to cause particle migration. The use of coupled fluid-particle DEM simulations explores this criterion in this research study. The geometric factors relate to the particle size distribution and fabric as discussed further below.

The mechanical factor considers the dependency of the initiation of erosion on the stress state, this is discussed further below and the issue of stress inhomogeneity is examined using the particle-scale data in the DEM simulations presented in later chapters.

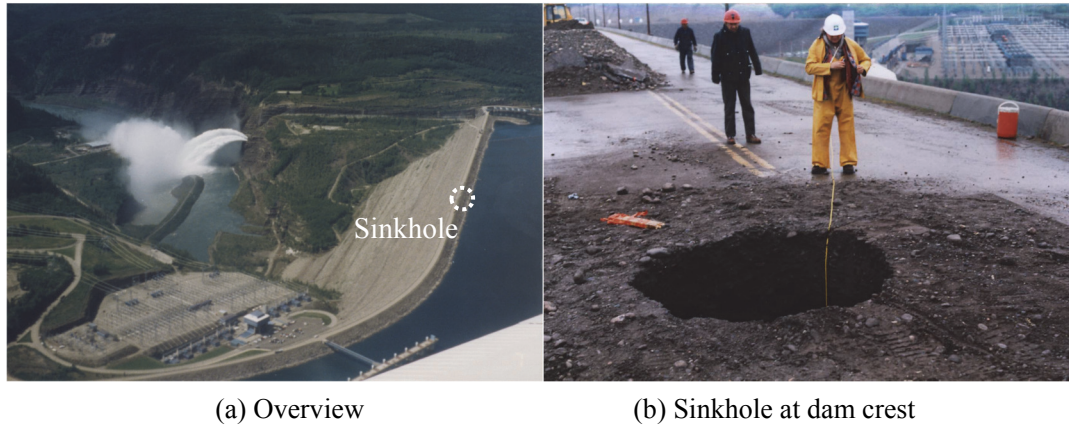


Figure 2.1 Sinkhole at WAC Bennett Dam in Canada in 1996 (Garner, 2006)

2.1.2. Internal instability

When soils are subject to internal instability, fine particles can move between coarse particles under seepage flow. It is thought that this happens specifically when fine particles are under relatively low stress as shown in Figure 2.2. Coarse particles are not detached and are responsible for transferring much of stress. According to ICOLD (2015), soils which are gap-graded, non-plastic and underfilled (i.e. when the fine particles are insufficient to fill pores between coarse particles) tend to be internally unstable.

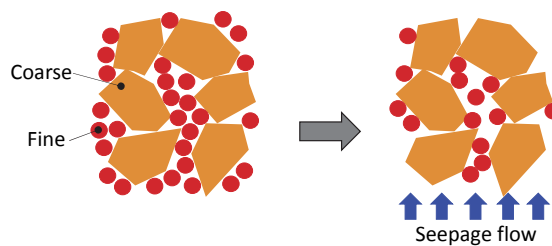


Figure 2.2 Schematic drawing of internal instability

In respect of the onset of erosion, filter criteria play an important role to determine whether soil particles are washed out, i.e. they are used to assess the vulnerability of a particular soil to internal instability. There are some widely used criteria such as those proposed by Kezdi (1979) or Kenney & Lau (1986). These criteria consider the shape of the particle size distribution (PSD). Kezdi (1979) proposed a geometric criterion for the assessment of internal instability using the ratio of D'_{15}/d'_{85} as illustrated in Figure 2.3. When gap-graded PSDs are considered, the PSDs

can be clearly divided into a coarse and fine fraction. The diameters of particles in the coarse fraction are represented by D' . 15% of coarser particles (by mass) are smaller than D'_{15} . The particle diameters in the fine fraction are represented by d' . 85% of the finer particles (by mass) are smaller than d'_{85} . For gap-graded soils, D'_{15}/d'_{85} is an index for considering susceptibility to internal instability. Soils with a ratio $D'_{15}/d'_{85} < 4$ are regarded as being internally stable. This concept was originally developed by extending the idea of Terzaghi & Peck (1948) for evaluating the ability of a uniform filter to prevent erosion of a cohesionless base material, commonly known as Terzaghi's filter criterion.

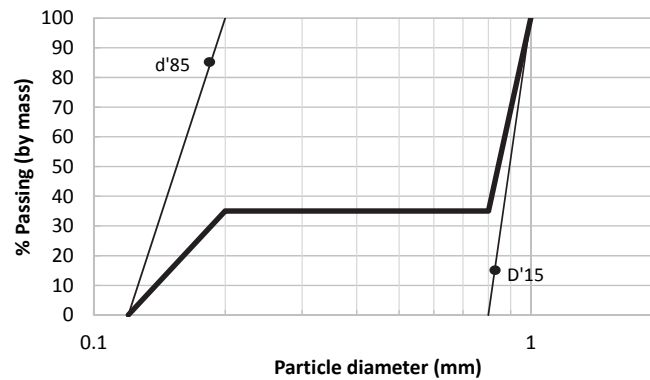


Figure 2.3 Kezdi criterion: Definition of gap ratio (D'_{15}/d'_{85})

Depending on the amount of fine particles, soils can be classified as underfilled or overfilled as shown in Figure 2.4. In an underfilled material the fines do not completely fill the voids between the coarse grains. In an overfilled material the fines completely fill the void space and separate the coarser grains. Skempton & Brogan (1994) found that for underfilled materials the fines content F_s is less than 24% to 29%, depending on porosity. They found that F_s is above 35% for overfilled materials. For transitional materials, which are between underfilled and overfilled, with $24\% < F_s < 35\%$, the extent to which the coarse and fine grains interact depends on the density level (Shire, 2014).

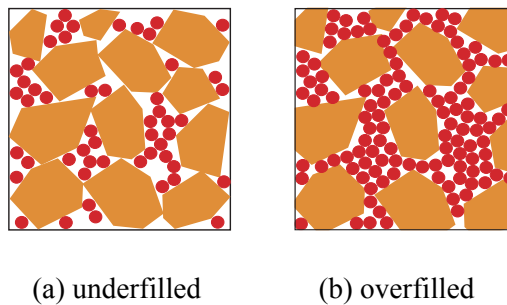


Figure 2.4 Schematic diagrams of soil state

According to Terzaghi's classical theory for heave, the critical hydraulic gradient in an internally stable soil is defined as hydraulic gradient where the effective stress becomes zero. In this situation, piping is expected to occur when the resultant body force is zero, i.e. gravitational forces are cancelled out due to upward seepage forces. On the other hand, the critical hydraulic gradient i_{crit} in an internally unstable soil is regarded as the point where the migration of fine particles is noticeable (Skempton & Brogan, 1994). As far as the work of Skempton & Brogan (1994) is concerned, the critical hydraulic gradient in vertical direction was at least three times lower than the theoretical critical hydraulic gradient for heave ($i_{crit,heave} \doteq \gamma'/\gamma_w \doteq 1$) for materials susceptible to internal instability, i.e. $i_{crit} < 0.3$.

2.2. Experimental studies on internal instability

Consideration of suffusion, which is one form of internal instability and is categorised in Figure 1.1, is central to this study. When suffusion takes place, the overall volume of soil does not change even though fine particles are eroded under seepage flow. This phenomenon occurs at a much lower hydraulic gradient than that calculated from the Terzaghi classic theory for heave (Terzaghi & Peck, 1948), which is called critical hydraulic gradient (Skempton & Brogan, 1994). ICOLD (2015) states that "As there are no generalized methods for accurately predicting the critical seepage gradient, laboratory tests should be carried out which carefully simulate the field conditions". In this section, research based on experiments is presented.

2.2.1. Hydraulic gradient and seepage velocity effects on the initiation of suffusion

The hydraulic gradient or seepage velocity causing suffusion is the most important factor considered here. Understanding which of these two parameters is critical is the subject of some controversy. Perzmaier (2007) summarised that hydraulic gradient cannot sufficiently justify the movement of particles, and the critical seepage velocity should be considered. Vogt et al. (2015) state that both hydraulic gradient and seepage velocity should be considered for safety evaluation of internal erosion in future versions of Eurocode7.

When fluid velocity within soil is considered, it is important to consider Darcy's law. Darcy in 1856 proposed an empirical equation for fluid flow through saturated soils. According to the work of Darcy, fluid flow through a cross-sectional area of soils under a particular hydraulic gradient can be specified as follows:

$$Q = kiA \tag{2.1}$$

where Q is the fluid flow, k is the coefficient of permeability, i is the hydraulic gradient, and A is

the cross-sectional area of soil. Note that Darcy's law assumes that fluid flow is laminar, the soil is saturated, and no change in void volume occurs. Continuity or mass conservation is also assumed. By using this Equation 2.1, the velocity of flow can be written as:

$$v_{discharge} = \frac{Q}{A} = ki \quad 2.2$$

where $v_{discharge}$ is the fluid velocity. The $v_{discharge}$ is the fluid flow per unit area of soil. The actual fluid velocity, however, is the flow in the voids. The seepage velocity ($v_{seepage}$) is defined as:

$$v_{seepage} = \frac{v_{discharge}}{n} \quad 2.3$$

where n is the porosity. Note that seepage velocity is always faster than discharge velocity since n is always smaller than 1. The seepage velocity is, however, not the actual fluid velocity in the voids. As illustrated in Figure 2.5, the actual velocity locally varies in the void space. Taylor (2016) obtained data on void space topology using micro computed tomography (μ CT). These data enabled computational fluid dynamics (CFD) simulations to get information on the local velocities and pressures of the fluid in the void space. Figure 2.6 is a representative result from his simulations and it is clear that while the median local velocity is close to the seepage velocity, there are a broad range of local velocity values, even for the laminar flow scenario considered by Taylor (2016).

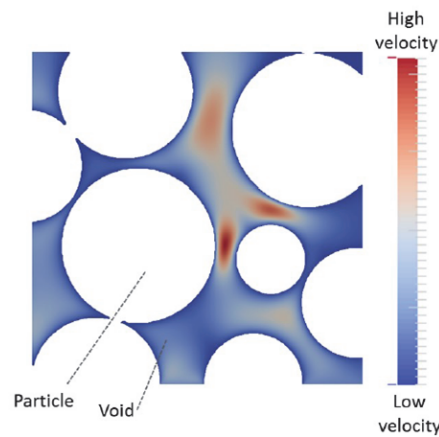


Figure 2.5 Qualitative contour maps of actual velocity magnitude (Taylor, 2016)

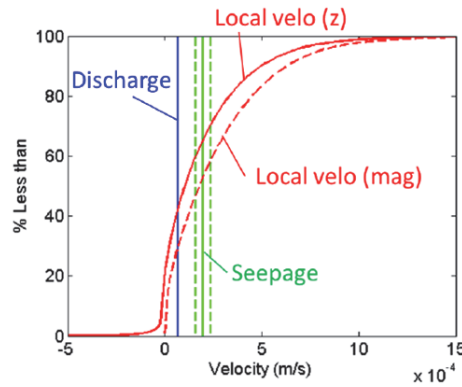


Figure 2.6 Cumulative distribution function for discharge, seepage and actual velocities for sand with $C_u = 3$ (Taylor, 2016)

Richards & Reddy (2012) experimentally investigated the initiation of suffusion and backward erosion for different soils including gap-graded PSDs using a new true-triaxial piping test apparatus. The discharge velocity was monitored and there was a turbidimeter at the outlet port. When suffusion initiated, fine particles were washed out, and there was a transition from suffusion to backward erosion. Once suffusion happens, backward erosion occurred at a much lower discharge velocity than theoretically expected. They defined the velocity causing the onset of piping as the critical velocity. According to their results, the critical velocity was a better index for piping behaviour than the hydraulic gradient. An increase in pore water pressure and/or a reduction in confining pressure caused the decrease of the critical velocity for pipe initiation. Initial void ratio significantly influenced the critical velocity as well, meaning that the amount of fine particles play a significant role in piping initiation.

2.2.2. Overall stress state

The correlation between hydraulic gradient and effective stress where internal instability initiates is not clearly understood. The concept of a hydro-mechanical failure envelope in hydraulic gradient-stress space was proposed to quantify failure conditions by Moffat & Fannin (2011). The onset of seepage-induced failure with large deformations occurred at a specific combination of hydraulic gradient and effective stress. Permeameter tests with four widely graded cohesionless soils under unidirectional (upward and downward) seepage flow were carried out, and effective stresses ranging from 25 to 175 kPa were applied. A linear fit between the critical hydraulic gradient and vertical effective stress, which was independent from the seepage direction, was reported as a hydro-mechanical failure envelope as shown in Figure 2.7. Chang & Zhang (2013) also found that the critical hydraulic gradient causing the onset of suffusion increased linearly with mean normal stress level for isotropic stress states. Three type stress states were considered by Chang & Zhang (2013): isotropic stress, triaxial compression stress,

and triaxial extension stress. In the compression stress condition, the major principal stress is along the seepage flow direction, whereas the major principal stress is perpendicular to the seepage flow direction in the extension stress condition. Triaxial permeameter tests were carried out with a gap-graded soil. The results showed that the hydraulic gradient causing internal erosion was strongly linked to pore structure, i.e. porosity. As shown in Figure 2.8, the initiation hydraulic gradient i_{start} , which was defined as the hydraulic gradient that initiates internal erosion, under compression stress condition initially increased with the shear stress ratio but decreased at shear failure. This was attributed to the formation of elongated pores locally along the seepage flow direction. The hydraulic gradient under extensive stress was higher than that under compressive stress.

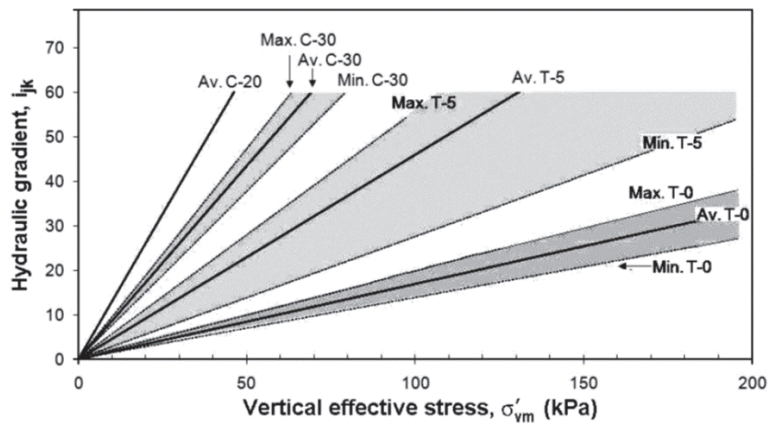


Figure 2.7 Hydro-mechanical relation (Moffat & Fannin, 2011)

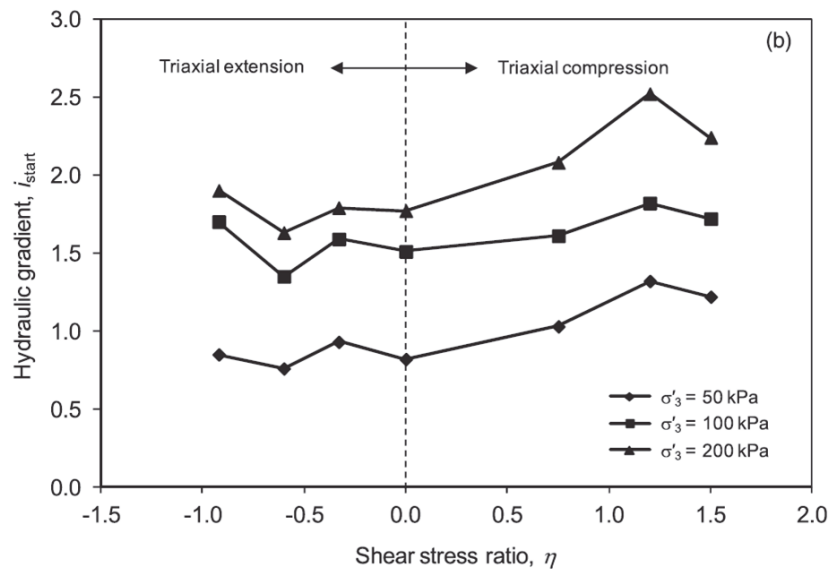


Figure 2.8 Hydraulic gradients causing internal erosion under various shear stress ratio (Chang & Zhang (2013))

2.2.3. Stress distribution within material

The stress distribution within the soil is important. Specifically, the amount of stress the fine particles transfer. This concept is a key contribution to evaluate the hydro-mechanical factor, which can be quantified by a reduction factor α originally proposed by Skempton & Brogan (1994). Using permeameter experiments as illustrated in Figure 2.9, it was empirically found that suffusion initiation in internally unstable soils occurred at much lower hydraulic gradients than the critical hydraulic gradient i_{crit} , which could be anticipated theoretically by means of Terzaghi's classic theory for assessing heave. This was attributed to the mechanism of stress transfer between the fine and coarse particles. Coarse particles were thought to be responsible for transferring most of stress through a matrix of contacting coarse particles, and the fine particles, which are sitting in the void space between the coarse particles, experienced relatively small stress. Li & Fannin (2008) also hypothesised that the reason for this may as well come from a reduction in stress of fine particles and the concept of stress reduction. Skempton & Brogan (1994) defined α as the ratio of the stress in the finer fraction $\overline{\sigma_{fine}}$ to the overall applied stress $\overline{P^P}$:

$$\overline{\sigma_{fine}} = \alpha \overline{P^P} \quad 2.4$$

where $\overline{\sigma_{fine}}$ is the mean normal stress acting in the finer particles; α is the stress reduction factor; and $\overline{P^P}$ is the mean normal stress for the entire system or sample.

Skempton & Brogan (1994) hypothesised that α could be estimated by considering the hydraulic gradient at which there was significant particle migration. Integrating the stress reduction factor with Terzaghi's classic theory, the critical hydraulic gradient for a cohesionless soil without stress applied on surface became:

$$i_{crit} = \frac{\alpha \gamma'}{\gamma_w} \quad 2.5$$

where i_{crit} is the critical hydraulic gradient; γ' is the buoyant unit weight; and γ_w is the unit weight of water. It was shown that hydraulic gradient causing the initiation of internal instability was smaller than that expected for heave.

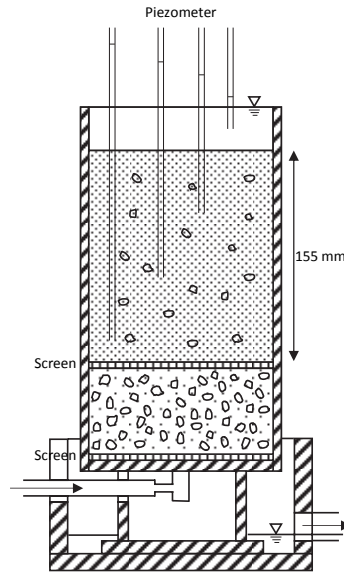


Figure 2.9 Apparatus for permeameter experiment (after Skempton & Brogan, 1994)

Moffat & Herrera (2014) used an index denoted G , which was a geometric-based stress reduction factor that determined the proportion of stress transferred to the particles of the fine soil particles like α , and compared the relationship between G and α , and the ratio (D'_{15}/d'_{85}) , which is explained in Section 2.1. It was shown that the decrease in the D'_{15}/d'_{85} increased G , which caused an increase in the critical hydraulic gradient. The values of α obtained independently from tests on cohesionless internally unstable soils follow a similar trend of G from results.

Slangen (2015) investigated the factors affecting internal instability for gap-graded soils under upward seepage flow using a double walled triaxial permeameter. In Slangen's work, all gap-graded soils were reconstituted by means of modified slurry deposition method and then isotropically compressed to 50 and 150 kPa. It was found that the micro-structure, i.e. void ratio and fines content, of specimens has an impact on the susceptibility of internal instability toward upward seepage flow. It is clearly shown that the proposed state parameter composed of void ratio is a good index of the relative susceptibility to suffusion.

2.3. Numerical approach toward internal instability

Understanding the suffusion process is a key contribution to assess the susceptibility to the onset of the suffusion under a specified hydraulic gradient and seepage velocity. Maeda et al. (2012) and Maeda & Kondo (2014) investigated the possibility of fine particle erosion causing deformation or failure of soils using DEM (without CFD coupling). In this study, suffusion was reproduced by removing fine particles as implemented in a previous paper (Muir Wood et al., 2010), and soil behaviour before and after suffusion occurred was investigated. However, the

initiation of the suffusion was not considered only the consequences. In fact, no DEM study looking at effects of overall applied stress and stress distribution under water flow was identified in the review of the literature carried out to support the current research. In this section, research based on numerical analyses is presented. Section 2.3.1 looks at DEM simulations of phenomena similar to internal instability. Section 2.3.2 looks at DEM analyses of stress inhomogeneity. Stress inhomogeneity is thought to be a major factor influencing susceptibility to internal erosion.

2.3.1. Simulation of internal erosion of granular filters with coupled DEM

After the fine particles are washed out from inside soils, suffusion is easily changed to piping, which is induced by regressive erosion of particles from downstream. Vogt et al. (2015) propose that the Eurocode EC7 be modified to formally recognise that piping is a form of failure by internal erosion. El Shamy & Aydin (2008) investigated flood-induced piping in river levees using uniformly graded spherical soil particles. They used the PFC3D code (version 3.1) with the CFD coupling feature that was implemented in that version of PFC3D. In this study, a link between particle movements and the increments in seepage forces was observed. Figure 2.10 gives data for porosity and critical hydraulic gradient close to the downstream as a function of the applied difference in head. The critical hydraulic gradient considered here is Terzaghi's theoretical gradient rather than a value measured from the DEM simulation. The change in porosity at hydraulic gradients lower than 1 indicates particle migration before piping conditions that would be calculated from Terzaghi's approach occur.

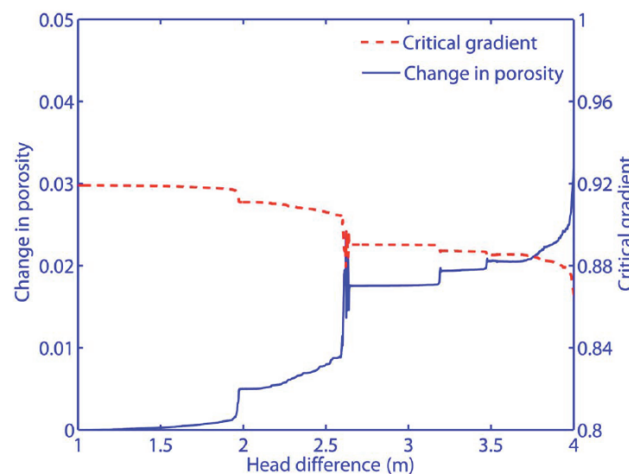


Figure 2.10 Effect of head difference on porosity and critical gradient (El Shamy & Aydin, 2008)

Jeyisanker & Gunaratne (2009) analysed seepage flow in a two-layer filter system under a controlled hydraulic gradient. Figure 2.11 is a schematic of the double-layered system that they

modelled. They validated their model using the Hazen (Equation 2.6) and Chapuis (Equation 2.7) expressions (Das, 2006) that relate permeability to void ratio and particle size. They compared local and global hydraulic gradients and found that the local hydraulic gradients could be much larger than the globally applied values. Compaction deficiency makes the pore pressure distribution non-uniform, affecting local flow and hydraulic gradient, as shown in Figure 2.12.

Hazen	$k = cD_{10}^2$	2.6
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Chapuis	$k = 2.4622 \left(D_{10}^2 \frac{e^3}{1+e} \right)^{0.7825}$	2.7
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where c is the constant that varies from 1.0 to 1.5; D_{10} is the 10% passing particle diameter; and e is the void ratio. Note that the unit of k used here is cm/s, and the unit of D_{10} is mm.

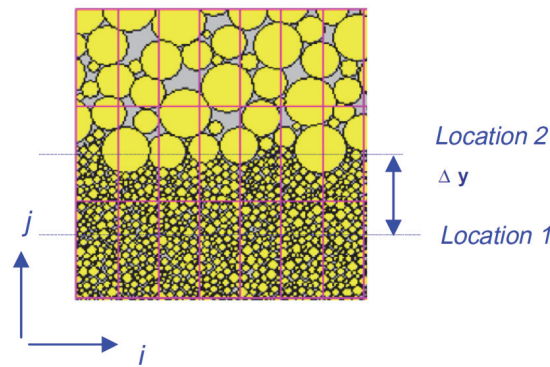


Figure 2.11 Illustration of localised hydraulic gradient (Jeyisanker & Gunaratne, 2009)

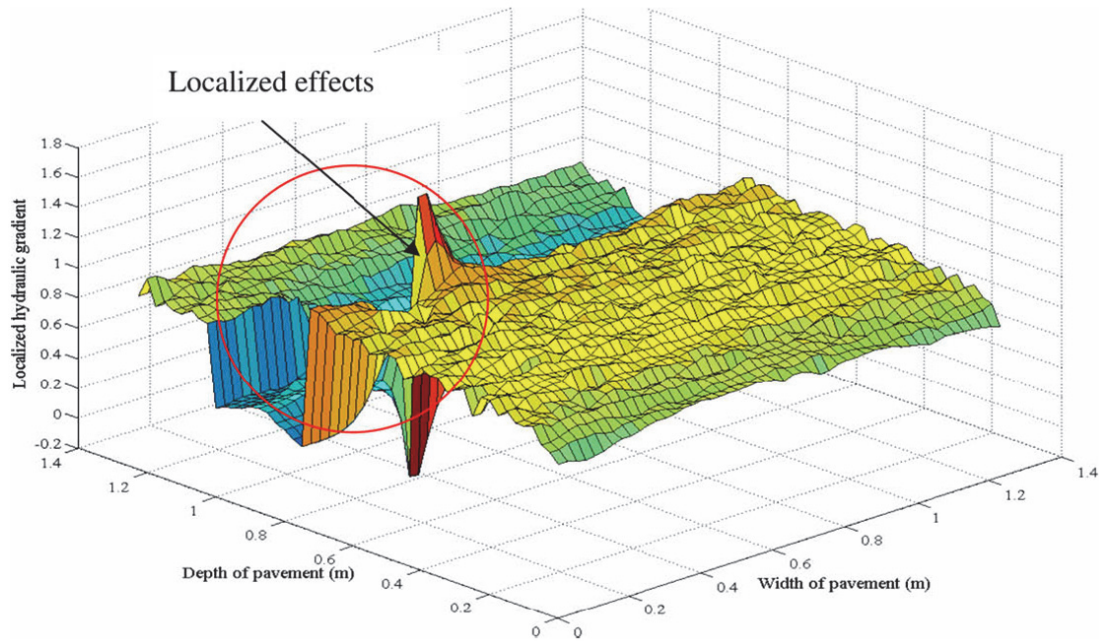


Figure 2.12 Plot of localised hydraulic gradient (Jeyisanker & Gunaratne, 2009)

Kim & Whittle (2009) observed the simulation of filtration mechanisms considering a quasi 1D network model as illustrated in Figure 2.13 to the filtration of a microfine cement suspension injected through a column filled with sand. They called their model a bubble model. This model considers migration of particles in a cylindrical pore by applying a version of Stoke's law. This model also appears to be a more sophisticated version of the network model proposed by Shire (2014). It was found that detachment rate determined effluent concentration and spatial distribution of filtered particles within the soil.

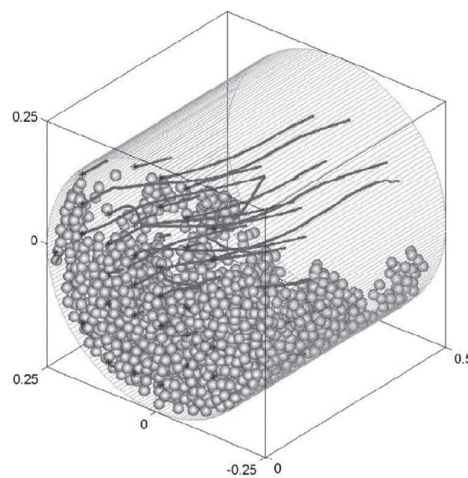


Figure 2.13 Illustration of particle migration (Kim & Whittle, 2009)

Sari et al. (2011) observed the internal erosion process of granular beds subjected to upward or downward seepage flow using the Yade DEM code. They described their fluid phase model as being a pore-scale discretisation of Stoke's equations, where pores were defined by tetrahedral cells resulting from the regular Delaunay tessellation of the sphere packings. All their simulations looked at the interaction between a finer base layer and a coarser filter flayer. Three configurations were considered: a sample with completely separated fine and coarse particles under downward flow (base-filter relationship), a sample with mixed fine and coarse particles without flow (segregation), and a sample with mixed fine and coarse particles under upward flow (suffusion). In particular, the last sample, shown in Figure 2.14, was useful to consider particle migration under gravity and fluid flow. In terms of this sample, suffusion of fine particles was observed once the imposed pressure or fluid flow was sufficiently large. When pressure was applied from the bottom, there was a threshold value of 10 kPa, i.e. for the case with imposed pressure of 10 kPa, a small cavity emerged, and the erosion process initiated. After the simulation had been running for some time, fluid flow abruptly increased, and the cavity size increased. Similarly, there was a threshold when an imposed fluid flow rate was applied. When erosion occurred in the pressure-controlled simulations, the imposed pressure could be stably controlled to maintain constant fluid flow. However, for the imposed fluid flow case, the pressure had to be adjusted to obtain a constant flux while internal erosion caused the increase of permeability, resulting in generating the fluctuation of both fluid flow and pressure for a while.

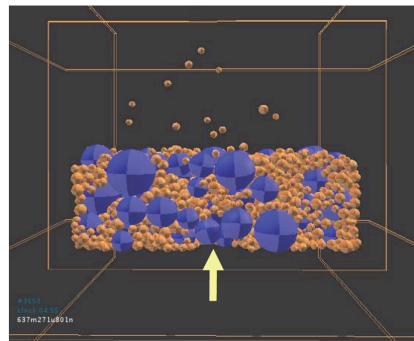


Figure 2.14 Packing subjected to upward seepage (Sari et al., 2011)

Zou et al. (2013) observed the mechanism of particle transport into four types of granular filters as shown in Figure 2.15, simulating clay, fine sand, coarse sand, and gravel. This study used the particle flow method, which was probably the PFC3D, to simulate particle transport, and fluid-particle interaction was considered using the Navier-Stokes equations. Again, they considered the interaction between a finer base material in a coarser filter material. The distribution of eroded particles, which ranged in number from 50 to 6,000, was traced and intruded depth into

granular filters was analysed under varying calculation time and hydraulic gradients. It was found that filters with the gap ratio < 4 , i.e. Figure 2.15 (a) and (b), was effective for protecting particles from seepage erosion and eroded mass did not increase even under high hydraulic gradient and long simulation time, which was approximately 0.02 seconds. Although some research, e.g. Li & Fannin (2008), reported that gap ratio was not always good index for knowing about the susceptibility of soil particles to move with seepage flow, it was broadly accurate in this study.

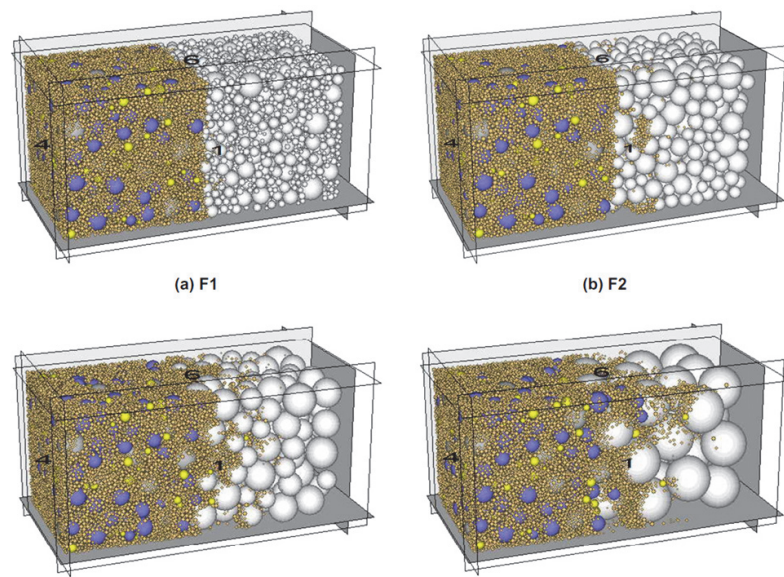


Figure 2.15 Distribution of eroded particles into filters (Zou et al., 2013)

Abdoulaye Hama et al. (2016) studied internal stability of widely graded materials and their mechanical behaviour after suffusion as shown in Figure 2.16. They used the PFD3D code (version 4.0) with the lattice boltzmann method for simulating fluid flow governed by the Navier-Stokes equations, which was linked to the PFC3D environment. Smaller particles' migration through throats between coarse particles under downward seepage flow was analysed in these materials. The materials were initially stable based on the criterion of Kenney & Lau (1986). However, fine particles, initially regarded as stable, were washed out due to downward seepage flow, and local instability was confirmed. It was confirmed that criterion defined by Kenney & Lau (1986) did not always appear to be effective as it was observed by Zou et al. (2013) and indicated that fines contents were quite important to verify whether soil was stable or unstable.

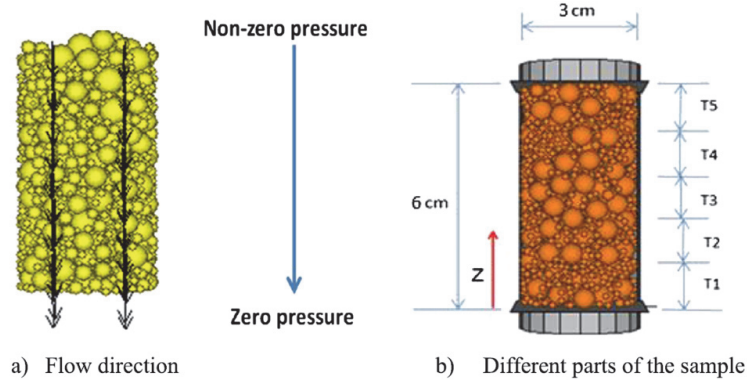


Figure 2.16 Simulation samples (Abdoulaye Hama et al., 2016)

2.3.2. Heterogeneity of stress distribution in granular materials

In a DEM model, the stress distribution within a numerical sample can be studied as all the particles can be individually traced, and detailed information about each particle can be found. Shire et al. (2014) used DEM to revisit samples that were experimentally tested by Skempton & Brogan (1994) and Li & Fannin (2008), and largely confirmed the hypothesis that α gives an indication of particle-scale stress. Shire et al. (2014) directly calculated α rather than inferring it from hydraulic gradients at which particles started to move. To calculate α , the expression for an average stress tensor within a particle given by Potyondy & Cundall (2004) was used:

$$\overline{\sigma}_{ij} = \frac{1}{V} \sum_1^N \overline{\sigma}_{ij}^p V_p \quad 2.8$$

$$\overline{\sigma}_{ij}^p = \frac{1}{V_p} \sum_{c=1}^{N_{c,p}} f_j^c (x_i^c - x_i^p) \quad 2.9$$

where $\overline{\sigma}_{ij}$ is the stress tensor acting throughout the volume including particles and their surrounding void space; V is the total volume (particles + voids); N is the number of particles; $\overline{\sigma}_{ij}^p$ is the stress tensor in particle p ; V_p is the volume of particle p ; $N_{c,p}$ is the number of contacts on particle p ; f_j^c is the contact force transmitted at contact position x_i^c and x_i^p is the centroidal position. Using Equation 2.8, stress tensor for fine particles is given as follows:

$$\overline{\sigma}_{fine} = \frac{(1-n)}{\sum_{N_{p,fine}} V_p} \sum_{p=1}^{N_{p,fine}} \overline{\sigma}_{ij}^p V_p \quad 2.10$$

where $\overline{\sigma_{fine}}$ is the stress tensor acting in the finer particles; n is the sample porosity and $N_{p, fine}$ is the number of fine particles. In agreement with hypotheses put forward by Skempton & Brogan (1994), Shire et al. (2014) stated that the finer grains at the fines content of less than 24% did not completely fill void space between coarser particles, and thus fine particles carried little stress, and so that the material could be considered to be underfilled. At fines content above 35%, where the finer particles separated the coarser particles, fine particles transmitted significant stress, and the material could be considered as an overfilled condition. For transitional fines contents between 24 % and 35 %, the DEM data highlighted that the susceptibility to internal instability was very sensitive to packing density, i.e. relative density. Shire et al. (2014) found that typically $\alpha < 0.4$ for underfilled materials, while typically $\alpha > 0.8$ for overfilled materials. These conclusions were developed for isotropic stress and fabric and it was not clear whether they were applicable to more general stress states and fabrics.

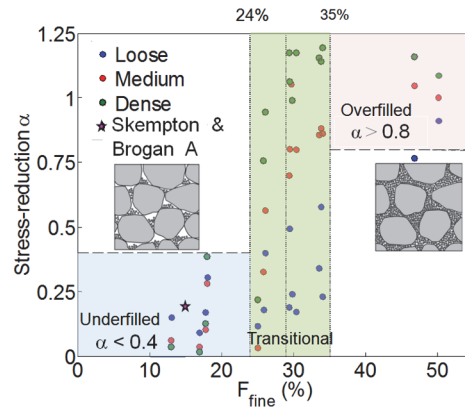


Figure 2.17 Variation in α with fines content (Shire et al., 2014)

Farahnak Langroudi et al. (2013) studied the stress transmission through internally stable and unstable gap-graded soils (Figure 2.18) under isotropic compression up to 4,000 kPa using DEM, providing an insight into micromechanical behaviour such as the suffusion of gap-graded soils. It was found that the internally stable assembly had a higher coordination and mechanical coordination number, whereas internally unstable assembly had more floating particles. The coordination number is the number of contacts per particle, while the mechanical coordination number is an adjusted measure, so only particles with two or more contacts are considered (Thornton, 2000). Accordingly, contact force chains were homogeneously distributed in the stable assembly in comparison with unstable assembly. In particular, more weak contact force existed in unstable assembly. In the unstable assembly, most of the stress was carried through coarse particles that comprised strong contact force chains, and stress reduction factor did not change very much even though applied pressure increased. In comparison with the work of

Shire & O’Sullivan (2013) and Shire et al. (2014), there are some samples with similar a fines content and a gap ratio. Although samples are different, the data on void ratio and stress reduction studied by Shire et al. (2014) seem to be in good agreement with results in the work of Farahnak Langroudi et al. (2013).

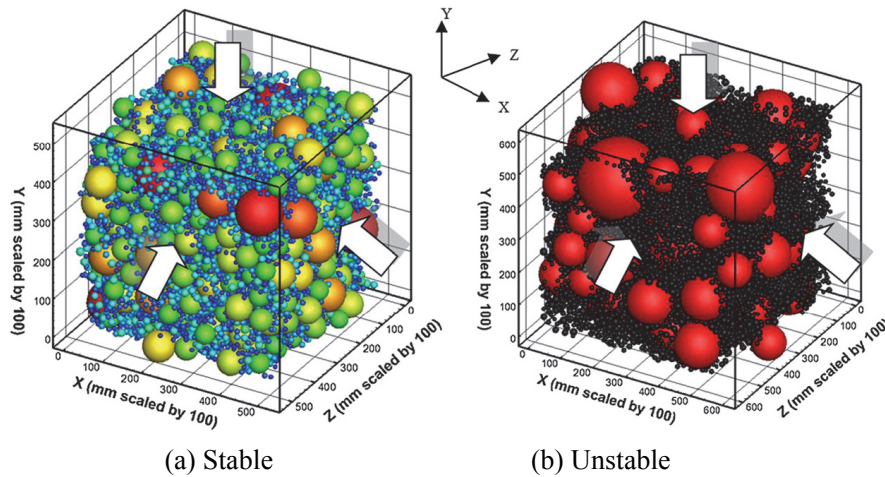


Figure 2.18 Gap-graded soil samples (Farahnak Langroudi et al., 2013)

2.4. Conclusions

Internal instability is a phenomenon that effects geotechnical structures. Initiation occurs at the particle scale, and interlinked hydraulic stress and material factors influence initiation. Some authors have speculated that seepage velocity governs the initiation of erosion, but most experimental research has emphasised that the link between stress state and the hydraulic gradient, where erosion initiates. Experimental researchers have provided particle-scale explanations that lack a scientific basis. Most prior DEM simulations looking at erosion and filters have considered base-filter interaction. There is clearly scope to advance knowledge of internal instability using coupled DEM-CFD modelling.

Chapter 3. DEM MODEL DEVELOPMENT

3.1. Introduction

The main focus of this research is coupled discrete element method (DEM) - computational fluid dynamics (CFD) simulations to study internal instability. The first step in the simulation process was to create samples to test in the virtual permeameter model that is discussed in Chapter 4. This step involves only DEM simulations and this Chapter explains how these simulations were carried out and presents preliminary results. Section 3.2 discusses the particle size distribution used. Section 3.3 explains how the samples were created. Section 3.4 characterises the samples at both macro and particle scales. A preliminary assessment of the methodology and data presented in this Chapter was given in the work of Kawano et al. (2016). The basic DEM algorithm is well documented in the literature and so it is not described here. Note however that this research used PFC3D version 5.00.21 and so PFC3D input scripts developed in prior research at Imperial College London, e.g. Cheung (2010) and O'Donovan (2014), could not be reused and significant coding was required.

3.2. Particle size distribution

The samples considered have a gap-graded PSD with 25% and 35% fines as illustrated Figure 3.1 (a) and (b) respectively. These PSDs were previously considered by Shire (2014) and Shire et al. (2014). The gap-graded PSD with 35% is given the greatest consideration in Chapter 5. Kezdi (1979) proposed that the internal stability of gap-graded soils can be assessed using the gap ratio $\frac{D'_{15}}{d'_{85}}$, where D'_{15} stands for the coarse fraction diameter for which 15% of coarse particles are smaller, and d'_{85} represents a fine fraction diameter for which 85% of fine particles are smaller as shown in Figure 3.1. In this approach, gap-graded soils are regarded as being internally stable if $\frac{D'_{15}}{d'_{85}} < 4$. Referring to Figure 3.1, in the current study particles exceeding 0.8 mm in diameter are considered to be coarse particles, while particles less than 0.2 mm are considered to be fine particles. $\frac{D'_{15}}{d'_{85}}$ of this gap-graded soil considered here is 4.6, meaning that this soil is on an unstable borderline, i.e. the soil may be susceptible to internal instability according to the Kezdi (1979) approach. As well as looking at the gap ratio, it is also important to consider the fines content as highlighted by Skempton & Brogan (1994) and Shire et al. (2014) as shown in Figure 3.2. Referring to Figure 3.2, Shire et al. (2014) showed that the stress in the finer fraction

depends on the fines content. As discussed in Chapter 2, when fines carry low effective stress, the material is more susceptible to internal instability. When a material is underfilled, the finer particles do not completely fill the voids between the coarser particles, and they have low stress. When a material is overfilled, the finer particles separate the coarse grains. They transmit sufficient stress so that the material is less susceptible to erosion. At the fines content of 25% and 35% considered here, the material is just in the transitional zone as indicated in Figure 3.2. In the transitional zone, the stress carried by the fines is very dependent on density (Shire et al., 2014).

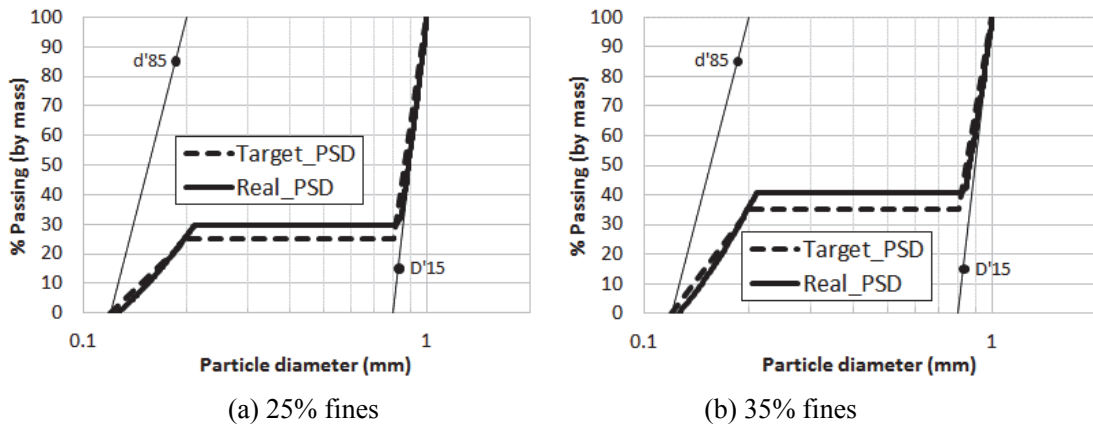


Figure 3.1 Target and real gap-graded PSD (note that d'_{85} : diameter at 85% passing in fine fraction and D'_{15} : diameter at 15% passing in coarse fraction)

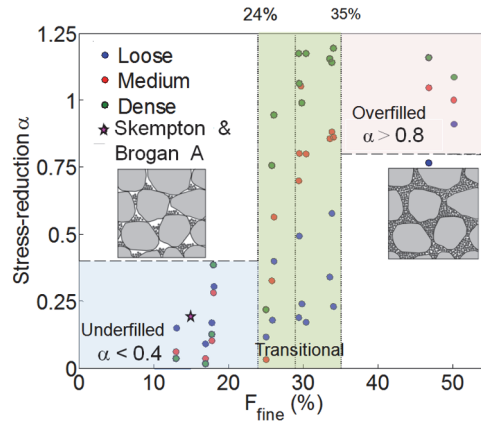


Figure 3.2 Variation in α with fines content (Shire et al., 2014)

3.3. Sample preparation method

In order to create DEM samples, two methods of sample preparation were adopted: compression and pluviation. Both methods were used with a rigid wall as rigid wall boundaries are necessary for coupling with CFD. Three coefficients of friction (μ) were used to control the

initial void ratio and relative density, so that $\mu = 0.0$ gave the densest samples, $\mu = 0.1$ gave medium-dense samples and $\mu = 0.3$ gave loose samples. Previous research has used various μ to control packing density including Shire et al. (2014) and Huang et al. (2014), and these were the μ values used in Shire (2014). Key DEM simulation parameters are given in Table 3.1; they are similar to the values for spherical glass beads used by Barreto (2008). DEM simulations are conditionally stable and the simulation time step is calculated as (Itasca Consulting Group, 2007):

$$t_{simulation} = \sqrt{\frac{m}{k_n}} \times \beta \quad 3.1$$

where $t_{simulation}$ is simulation time step; m = mass; k_n is spring constant (contact normal direction); and β is 0.25 (this is a safety factor which reduces the time step below the critical value calculated using the theory described by Itasca Consulting Group (2007)).

Table 3.1 DEM input parameters

Parameter	Value
Particle density, ρ	2.670 kg/m ³
Poisson's ratio, ν	0.3
Shear modulus, G	27.0 GPa
Coefficient of friction, μ	
between particle and particle	0.3
between particles during sample preparation	0.0, 0.1, 0.3
between particles and walls	0.0
Local damping	
during compression	0.10
during applying gravity	0.05
Gravity, g	9.80665 m/s ²
Time step, Δt	2.0E-8 s
Contact model	Non-linear Hertz-Mindlin
Boundary condition	Rigid wall

3.3.1. Compression

The particle assembly was firstly compressed under an isotropic confining stress and then gravity was applied. The process is shown in Figure 3.3. The compressed samples with 35% fines are illustrated in Figure 3.4; in this case, three numerical samples were prepared to consider

size effects on the sample properties. The samples had differing numbers of particles, the small sample had 3,315 particles (Figure 3.4 (a)), the medium sample had 15,982 particles (Figure 3.4 (b)), and the large sample had 31,793 particles (Figure 3.4 (c)). The equivalent sample considered by Shire et al. (2014) had 50,357 particles and used periodic boundaries. Three types of sample were created; loose samples with a coefficient of friction (μ) of 0.3, medium-dense samples with a coefficient of friction (μ) of 0.1, and dense samples with a coefficient of friction (μ) of 0.0. The compressed sample with 25% fines was also considered here, which had 19,790 particles with a coefficient of friction (μ) of 0.3 (loose sample) and a coefficient of friction (μ) of 0.0 (dense sample). The equivalent sample considered by Shire et al. (2014) had 36,928 particles and used periodic boundaries. Shire (2014) and Huang et al. (2014) amongst others showed that interparticle friction can be used to control density in DEM samples.

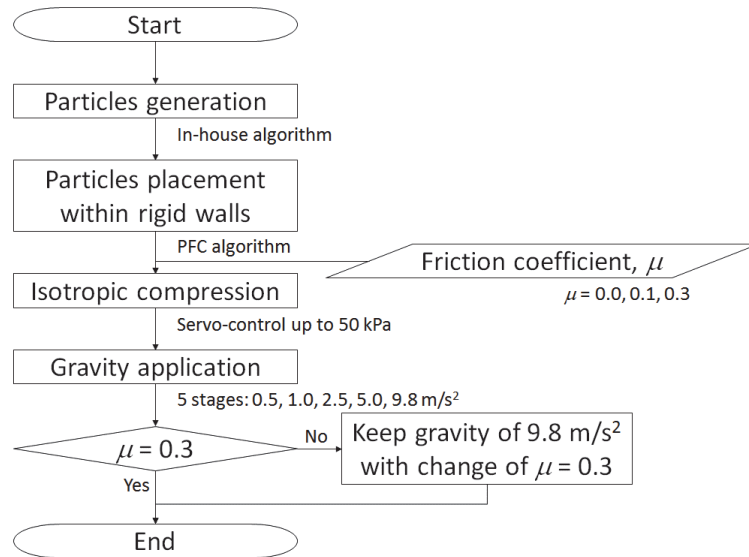


Figure 3.3 Flowchart of compression process

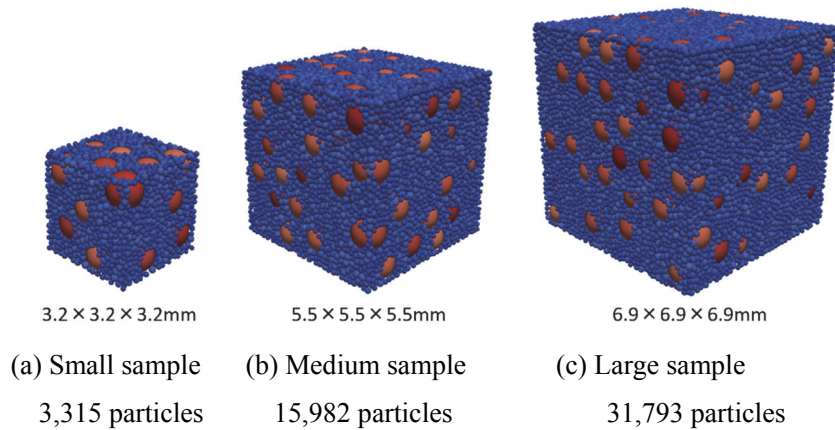


Figure 3.4 Schematic figures of three compressed numerical samples

As shown in Figure 3.3, to prepare the compressed samples, the particles were randomly placed in non-touching positions within a cubic container with rigid wall boundary conditions. The particle radii were selected to match the gap-graded PSD (Figure 3.1) by means of an in-house algorithm implemented in MATLAB. Then, the particles were placed in the cubic box using the PFC3D particle generation algorithm. The drawback of using the PFC3D algorithm is that the resultant particle assembly is inhomogeneous. There is a relatively large concentration of fine particles close to the rigid walls. This inhomogeneity arises because the algorithm is designed to place the particles in random positions where particles cannot overlap the rigid walls. This situation, however, is appropriate for considering real phenomenon since the conditions close to boundaries in laboratory experiments are similar to this situation, which is numerically created.

Each sample was isotropically compressed to mean effective stress of $p' = 50$ kPa. A local damping of 0.1 was applied to the simulations in order to minimise dynamic effects, and a stress-controlled servo-control algorithm was used during this compression stage. This algorithm applied a controlled strain rate that was gradually reduced as the target isotropic stress of $p' = 50$ kPa was approached. The variation in the strain rate imposed with stress is given in Figure 3.5. The target isotropic stress was measured on the walls. After the target isotropic stress was reached, and coordination number remained stable for a specific time, e.g. 500,000 steps (0.4 seconds in numerical time), the isotropic compression stage was terminated. Note that the coordination number is defined as the number of contacts per particle:

$$Z = \frac{2 \times N_c}{N_p} \quad 3.2$$

where Z is coordination number; N_c is total number of contacts; and N_p is number of particles.

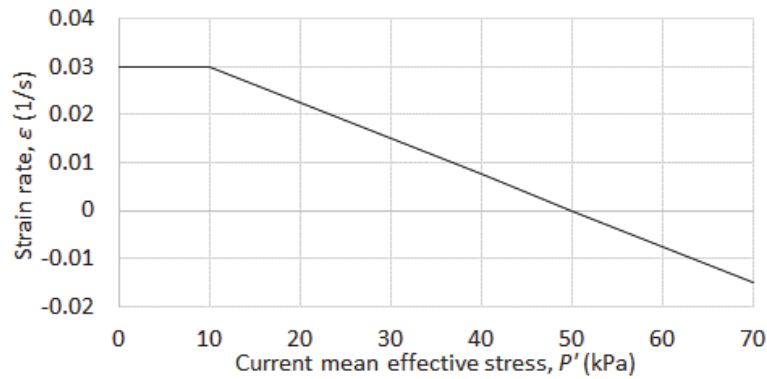


Figure 3.5 Strain rate applied in accordance with current stress

Gravity was gradually applied to all particles once the target isotropic stress of $p' = 50$ kPa was reached. Gravity was increased in five stages: 0.5, 1.0, 2.0, 5.0 and 9.8 m/s². This staged approach was adopted to avoid the significant impact forces that would occur due to a rapid change in contact forces if gravity was applied in one stage. The next increment of gravity was applied to the sample once the coordination number stabilised at each gravitational loading stage. Table 3.2 lists key sample properties including initial porosity (n_{ini}), porosity (n), coordination number (Z) and mechanical coordination number (Z_{mech}) at the end of gravitational loading stage, where the total volume of the sample surrounded by the rigid walls was considered. The mechanical coordination number Z_{mech} given in Table 3.2 was defined by Thornton (2000):

$$Z_{mech} = 2 \times \frac{N_c - N_p^1}{N_p - (N_p^1 - N_p^0)} \quad 3.3$$

where N_p^0 is number of particles with no contacts; and N_p^1 is number of particles with one contact. Note that contacts between balls and walls are not taken into account in Table 3.2.

3.3.2. Pluviation

A pluviated sample with 31,793 particles (large samples with 35% fines) was also prepared to consider segregation effects as shown in Figure 3.6. An initial sample size is the same as the compressed sample with 31,793 particles as shown in Figure 3.4 (c). In this case, all 31,793 particles fell under a gravitational body force, and compression was applied subsequently. Unlike the compression method as shown in Figure 3.3, samples are compressed up to the target stress of $p' = 50$ kPa after the gravity of 0.5 m/s² is applied as illustrated in Figure 3.7. Isotropic compression is not feasible because of dense fabric after a sample is pluviated under the gravity of 9.8 m/s². Just as for the compression method, the particles were randomly placed in non-touching positions using the in-house algorithm, and the gravity of 0.5 m/s² was initially applied. Once the simulation becomes stable, next stage of gravity was applied, and then the sample was compressed again up to 50 kPa in each stage. In each stage, the simulation continued until a steady state was reached, i.e. until the coordination number was stable for a specific time, e.g. 500,000 steps (0.4 seconds in numerical time). It took almost one week for each stage to reach a steady state. Once a gravitational acceleration of 9.8 m/s² had been achieved, and the sample was isotropically compressed up to 50 kPa, the simulation was terminated. The final sample properties are listed in Table 3.2 as sample “Pluviated-loose” and sample “Pluviated-dense”, where the sample density was varied by specifying different μ values as before.

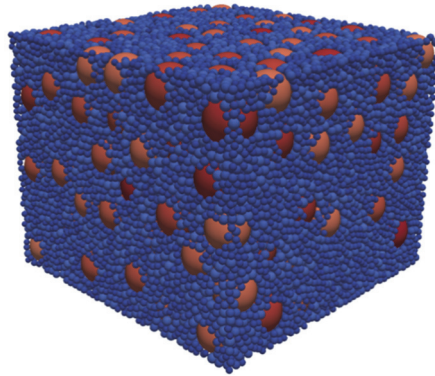


Figure 3.6 Schematic diagram of pluviated numerical sample: 31,793 particles

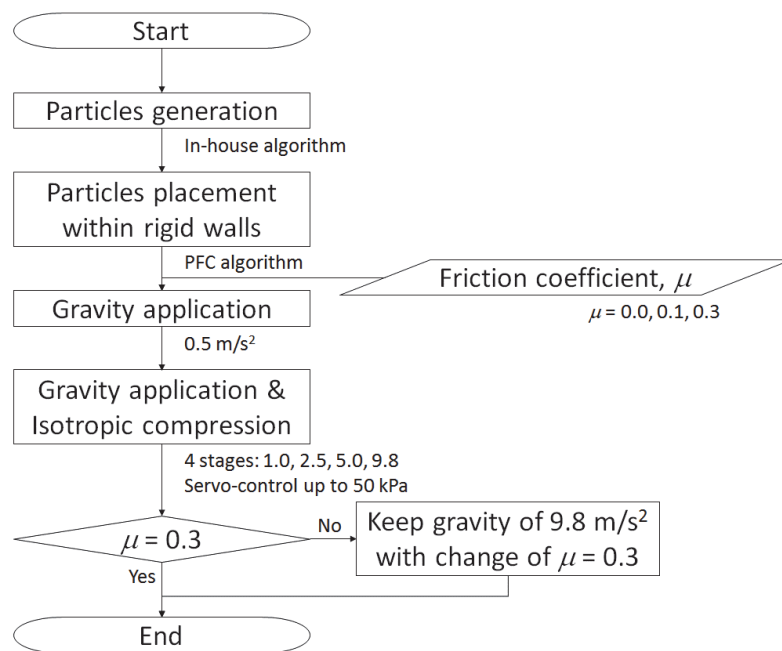


Figure 3.7 Flowchart of pluviation process

Table 3.2 Overall sample characteristics

Sample	Fines	Particles	Coarse	n_{ini}	μ	n	Z	Z_{mech}
Compressed								
Large-loose	25%	19,790	250	0.507	0.3	0.268	4.66	4.67
Large-medium					0.1	0.247	5.08	5.10
Large-dense					0.0	0.237	5.53	5.54
Small-loose	35%	3,315	25	0.480	0.3	0.298	4.49	4.52
Small-medium					0.1	0.292	4.82	4.84
Small-dense					0.0	0.281	5.25	5.26
Medium-loose	35%	15,982	125	0.496	0.3	0.283	4.65	4.66
Medium-medium					0.1	0.275	5.09	5.10
Large-loose	35%	31,793	250	0.491	0.3	0.278	4.69	4.70
Large-medium					0.1	0.271	5.17	5.18
Large-dense					0.0	0.257	5.67	5.68
Pluviated								
Large-loose	35%	31,793	250	0.491	0.3	0.280	4.69	4.70
Large-medium					0.1	0.271	5.16	5.17
Large-dense					0.0	0.257	5.68	5.69

From the data from Table 3.2, it is evident that porosity (n) becomes smaller with the reduction in coefficient of friction (μ) and that coordination number (Z) and mechanical coordination number (Z_{mech}) become larger with the increase of density. There is a clear correlation between the porosity and coordination number on samples with 35% fines content, i.e. an increase in coordination number is associated with a decrease in porosity as shown in Figure 3.8.

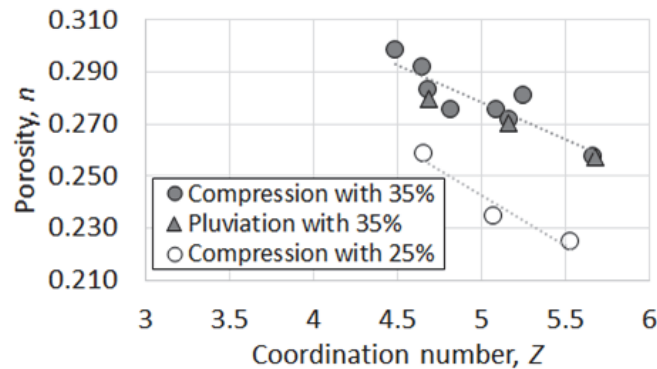


Figure 3.8 Correlation between porosity and coordination number

3.4. Evaluation of samples

3.4.1. Selecting measurement sphere

The rigid boundaries will influence the packing. Observations of boundary effects on porosity, strain and contact force distributions near rigid walls include Chan & Ng (1986), Marketos & Bolton (2009) and Huang et al. (2014). Therefore, a measurement sphere was used to look at a representative volume in the centre of the sample at the beginning of simulations, e.g. Cui & O'Sullivan (2006). In a PFC3D model, a lot of parameters, such as coordination number, porosity, stress, and strain, are defined with respect to a specified measurement volume. This measurement volume is a sphere and is referred to as a measurement sphere. Here, the idea of an RVE defined by Nemat-Nasser & Hori (1999) is useful when selecting a measurement sphere radius. According to Nemat-Nasser & Hori (1999), an RVE for a material point of a continuum mass is a material volume which is statistically representative of the infinitesimal material neighbourhood of that material point. An RVE must include a significantly large number of corresponding microconstituents of the RVE. Also, it must be statistically representative of the local continuum properties, i.e. it must be large enough not to change measured parameters, e.g. coordination number, porosity, stress and strain when its own size changes. To explore how to achieve a RVE using a measurement sphere, different measurement sphere radii for the compressed samples with 35% fines content were considered, ranging from 20, 100 and 200% of a median diameter (D_{50}) away from the boundaries so that the effect of the measurement sphere size can be compared. In this research, the D_{50} for the entire grading was assumed to be 0.5 mm. The values for n and Z were in the measurement sphere are denoted $n_{\text{meas,sphere}}$ and $Z_{\text{meas,sphere}}$. For each sample, the measurement sphere was located at the centre of a sample so that it did not intercept boundaries. A measurement sphere is a specified measurement volume that may be created within a sample as shown in Figure 3.9. A measurement sphere that is big enough may be regarded as an RVE when parameters within a measurement sphere are statistically representative of the whole sample. As Table 3.3 below shows, the measurement sphere size measurably influences porosities and coordination numbers for the smaller samples, whereas the data for the larger samples show less variation with measurement sphere size. The ratio of the measurement sphere diameter (D_{measure}) to D_{50} is also shown in Table 3.3. A measurement sphere which extended to a distance of 20% of D_{50} from the walls was used in the remaining calculations below.

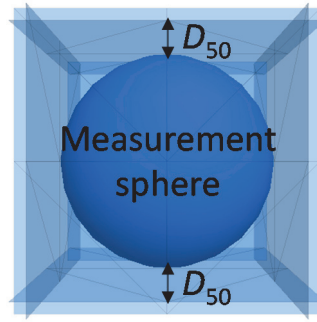


Figure 3.9 Schematic shape of measurement sphere

Table 3.3 Effect of measurement sphere size

Sample with 35% fines content	$D_{\text{measure}} / D_{50}$	Distance from walls	$n_{\text{meas,sphere}}$	$Z_{\text{meas,sphere}}$
Small-loose	2.5	20% of D_{50}	0.233	5.12
		100% of D_{50}	0.233	5.12
		200% of D_{50}	0.238	4.95
Large-dense	5.7	20% of D_{50}	0.222	6.11
		100% of D_{50}	0.223	6.09
		200% of D_{50}	0.224	6.07

Using a measurement sphere size that extends to 20% of D_{50} from the walls, final conditions are compared in Table 3.4. The data for “Gap Med 25” and “Gap Med 35” included on Table 3.4, come from the results of Shire et al. (2014) who used periodic boundaries and the same grading and used a different DEM code, LAMMPS (Plimpton, 1995). As expected, the denser samples have lower porosities and higher coordination numbers than the looser samples. In terms of the porosities, the results are in good agreement with Shire et al. (2014); however, there is a discrepancy in the coordination numbers. The absence of gravity in these earlier simulations allows particles to exist in a state of suspension in voids with no contacts, resulting in lower coordination numbers in comparison with the simulation data presented in Table 3.4. In respect of the pluviated samples, the porosity and coordination number are similar to the compressed samples.

Table 3.4 Final conditions within measurement sphere

Sample	Fines	Particles	Coarse	μ	$n_{\text{meas,sphere}}$	$Z_{\text{meas,sphere}}$
Compressed						
Large-loose				0.3	0.239	5.01
Large-medium	25%	19,790	250	0.1	0.211	5.52
Large-dense				0.0	0.201	6.12
Small-loose				0.3	0.233	5.12
Small-medium	35%	3,315	25	0.1	0.223	5.63
Small-dense				0.0	0.212	6.14
Medium-loose				0.3	0.243	4.92
Medium-medium	35%	15,982	125	0.1	0.233	5.49
Large-loose				0.3	0.244	4.90
Large-medium	35%	31,793	250	0.1	0.237	5.50
Large-dense				0.0	0.222	6.11
Pluviated						
Large-loose				0.3	0.252	4.91
Large-medium	35%	31,793	250	0.1	0.239	5.48
Large-dense				0.0	0.225	6.13
Shire et al. (2014)						
Gap Med 25-loose				0.3	0.258	0.15
Gap Med 25-medium	25%	36,928	500	0.1	0.224	3.09
Gap Med 25-dense				0.0	0.208	5.33
Gap Med 35-loose				0.3	0.245	3.08
Gap Med 35-medium	35%	50,357	500	0.1	0.241	4.62
Gap Med 35-dense				0.0	0.224	5.63

3.4.2. Evaluation of inhomogeneity

Each sample was divided into an integer number of layers to provide a layer depth of approximately 0.5 mm so that inhomogeneity in terms of porosity and PSD within the samples could be quantified. The approach used here was originally developed for cylindrical rigid-wall samples by Huang et al. (2014). The small samples were divided into six layers, the medium samples nine layers, and the large samples twelve layers. The ratio of layer thickness to maximum diameter D_{max} was fixed so that the effect of layer size can be neglected. This layering technique was adopted in the x, y, and z directions. The volume of each particle within each layer was accurately calculated by taking into account the intersection volume by means of determining the volume of the spherical cap, which is created when a sphere intersects a layer

boundary as shown in Figure 3.10. The corresponding volume is given in Equation 3.4:

$$V_{cap} = \frac{\pi h^2(3r - h)}{3} \quad 3.4$$

where V_{cap} = volume of spherical cap (hatched area in Figure 3.10); h = height of spherical cap; and r = radius.

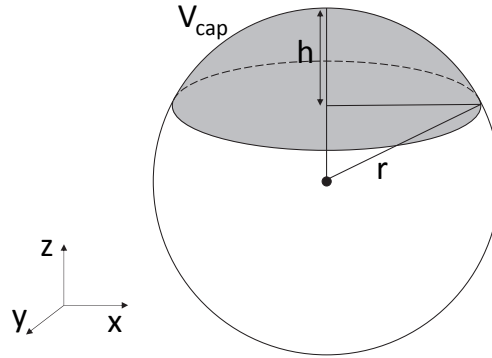


Figure 3.10 Schematic area of spherical cap

The detailed data for all samples considered are provided in Table 3.5 considering the vertical direction, which is the z direction. In addition to Table 3.5, the porosity distributions in all these coordinate directions are shown in Figure 3.11 to Figure 3.16. In each case, n values are normalised by the mean n excluding values in both end layers. It is clear that the porosity close to the top and bottom boundaries in all cases is higher than the average porosity in agreement with Chan & Ng (1986), Marketos & Bolton (2009) and Huang et al. (2014). There is also significant variation within the samples. The variation is more noticeable in the smaller samples, reflected in the higher standard deviation associated with these samples (Table 3.5). The greater variation in measured porosity in the layers in the smaller sample can simply be attributed to the fact that each layer is significantly smaller than an RVE. Therefore, the position and size of one particle within that layer can have a measureable influence on the porosity for that layer. Although the average porosity in Table 3.5 is not very different from the porosity within the measurement sphere in Table 3.4 especially for the larger samples, the difference between these results is still approximately 14%. Note that variability in the pluviated samples is higher than the compressed samples as listed in Table 3.5. This is probably due to local segregation.

Table 3.5 Porosity distribution of each layer in z direction

Layer No.	Large with 25% fines			Small with 35% fines			Medium with 35% fines		Large with 35% fines			Pluviated with 35% fines		
	Loose	Medium	Dense	Loose	Medium	Dense	Loose	Medium	Loose	Medium	Dense	Loose	Medium	Dense
Top layer														
1	0.329	0.317	0.303	-	-	-	-	-	0.343	0.341	0.328	0.331	0.342	0.329
2	0.265	0.240	0.217	-	-	-	-	-	0.253	0.240	0.226	0.241	0.228	0.218
3	0.251	0.228	0.224	-	-	-	-	-	0.269	0.264	0.251	0.281	0.276	0.260
4	0.278	0.245	0.232	-	-	-	0.321	0.318	0.265	0.262	0.246	0.260	0.247	0.239
5	0.264	0.228	0.219	-	-	-	0.269	0.252	0.264	0.255	0.243	0.272	0.261	0.244
6	0.259	0.236	0.227	-	-	-	0.270	0.266	0.267	0.262	0.249	0.270	0.257	0.247
7	0.263	0.230	0.230	0.325	0.325	0.320	0.284	0.274	0.257	0.252	0.237	0.264	0.255	0.240
8	0.250	0.228	0.217	0.278	0.268	0.254	0.259	0.254	0.268	0.257	0.245	0.268	0.259	0.245
9	0.268	0.253	0.237	0.283	0.278	0.268	0.281	0.274	0.277	0.274	0.257	0.278	0.261	0.246
10	0.238	0.219	0.215	0.299	0.286	0.271	0.265	0.256	0.271	0.264	0.248	0.292	0.281	0.266
11	0.248	0.236	0.227	0.254	0.246	0.238	0.267	0.256	0.259	0.249	0.235	0.252	0.235	0.222
12	0.307	0.303	0.295	0.351	0.346	0.333	0.329	0.328	0.337	0.334	0.322	0.348	0.344	0.332
Bottom layer														
Porosity	0.268	0.247	0.237	0.298	0.292	0.281	0.283	0.275	0.278	0.271	0.257	0.280	0.271	0.257
Excluding top & bottom														
Mean, μ	0.258	0.234	0.225	0.279	0.270	0.258	0.271	0.262	0.265	0.258	0.244	0.268	0.256	0.243
Standard deviation, σ	0.012	0.010	0.007	0.019	0.017	0.015	0.009	0.009	0.007	0.010	0.009	0.015	0.016	0.015

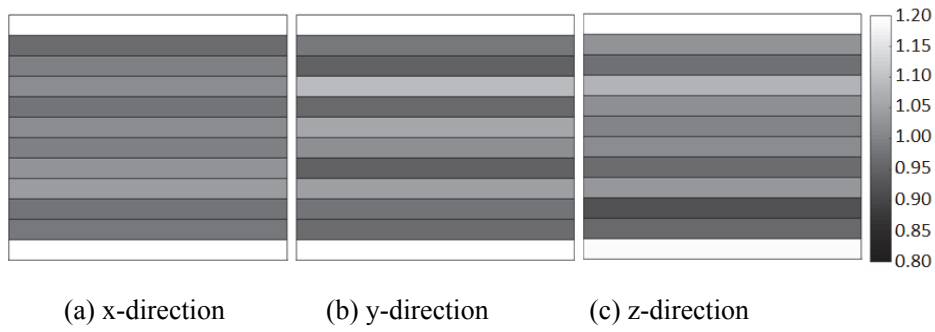


Figure 3.11 Normalised distribution of porosities in large-loose sample with 25% fines

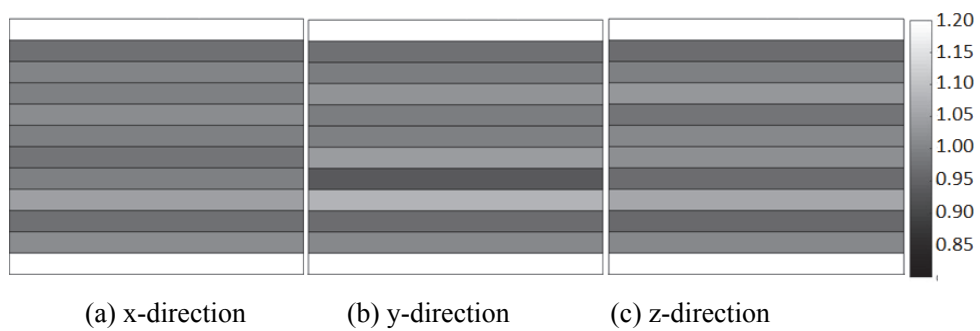


Figure 3.12 Normalised distribution of porosities in large-dense sample with 25% fines

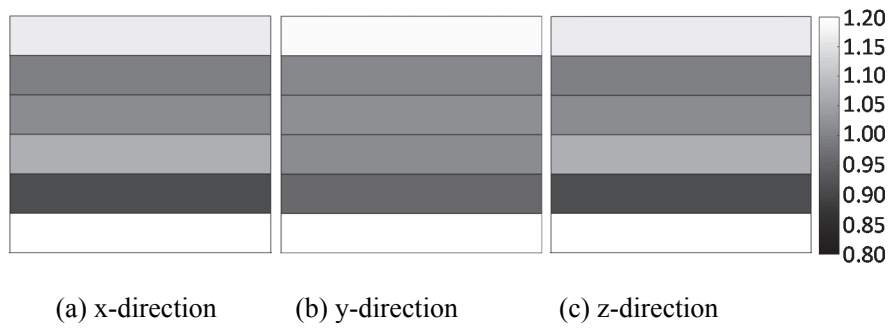


Figure 3.13 Normalised distribution of porosities in small-loose sample with 35% fines

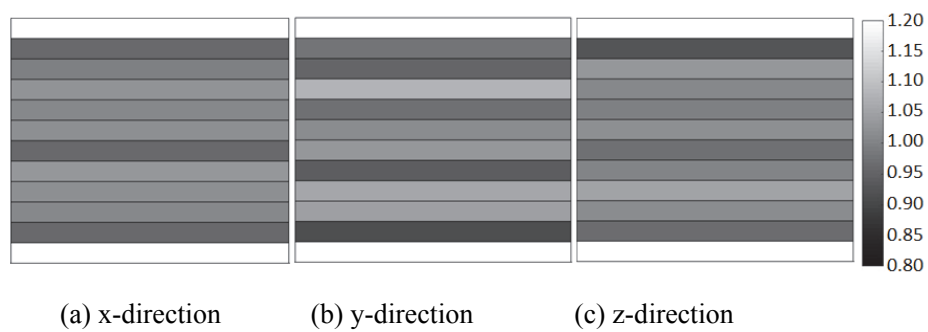


Figure 3.14 Normalised distribution of porosities in large-dense sample with 35% fines

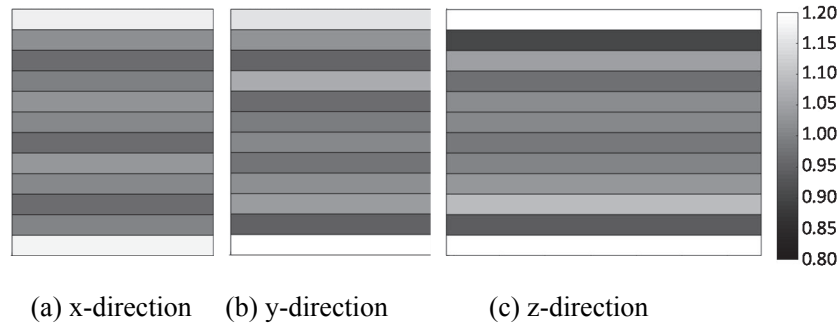


Figure 3.15 Normalised distribution of porosities in pluviated large-loose sample with 35% fines

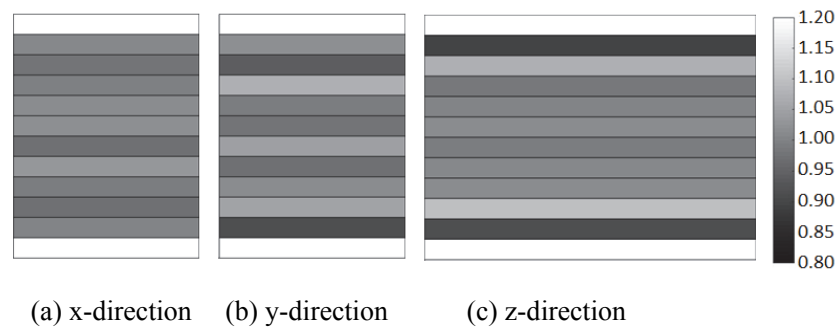


Figure 3.16 Normalised distribution of porosities in pluviated large-dense sample with 35% fines

The PSDs in each layer were compared to better understand the inhomogeneity as shown in Figure 3.17 to Figure 3.22. While there is some evidence of segregation in the small-loose sample with 35% fines (Figure 3.19), the samples with 25% fines have similar PSD trends in each layer (Figure 3.17 and Figure 3.18), and the PSDs of the large-dense and pluviated samples with 35% fines are very similar to each other, excluding the top and bottom layers (Figure 3.20 to Figure 3.22). Accordingly, these samples with 25% and 35% fines can be regarded as being homogeneous, meaning there is minimal segregation.

As Figure 3.20 illustrates, for the large-dense sample with 35% fines, more fine particles tend to be placed in bottom and top layers due to the effect of rigid walls. This is even more pronounced for the pluviated samples with 35% fines as shown in Figure 3.21 and Figure 3.22. It seems here that some of these fine particles must have fallen through the constrictions or pore throats in the void space between the coarse particles. Note also that the PSDs of layers No. 1 (top layer) and No. 12 (bottom layer) are broadly similar in this case.

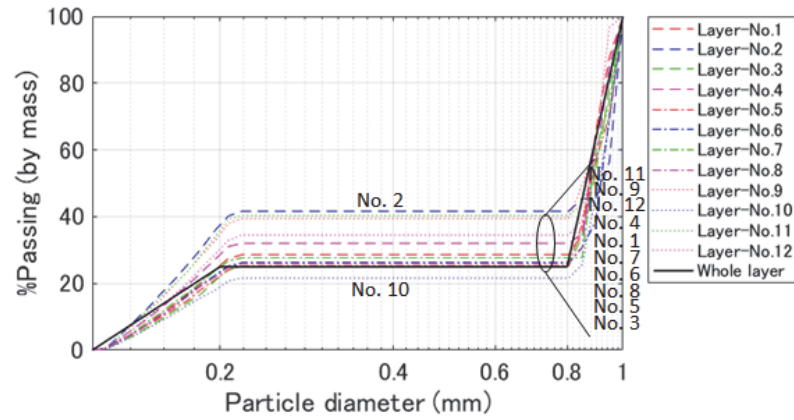


Figure 3.17 PSDs in each layer of large-loose sample with 25% fines

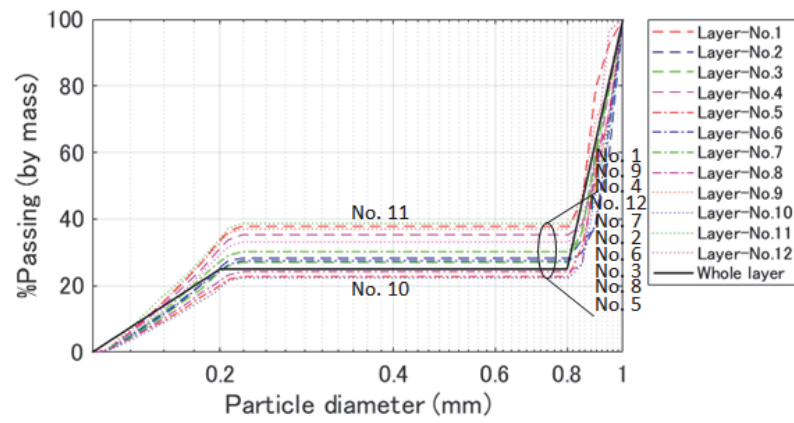


Figure 3.18 PSDs in each layer of large-dense sample with 25% fines

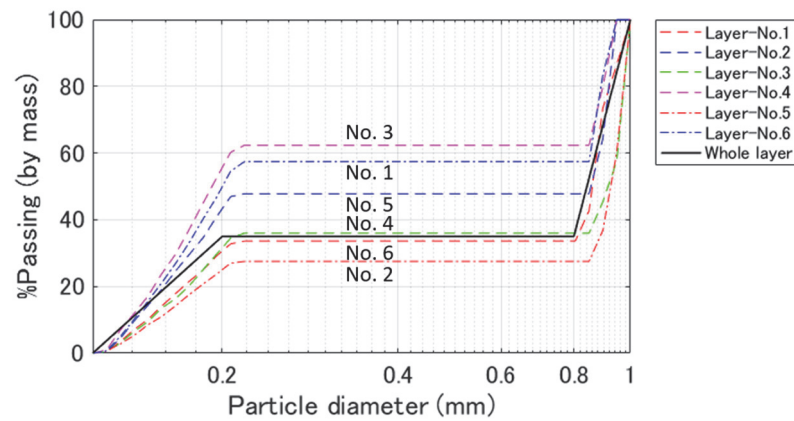


Figure 3.19 PSDs in each layer of small-loose sample with 35% fines

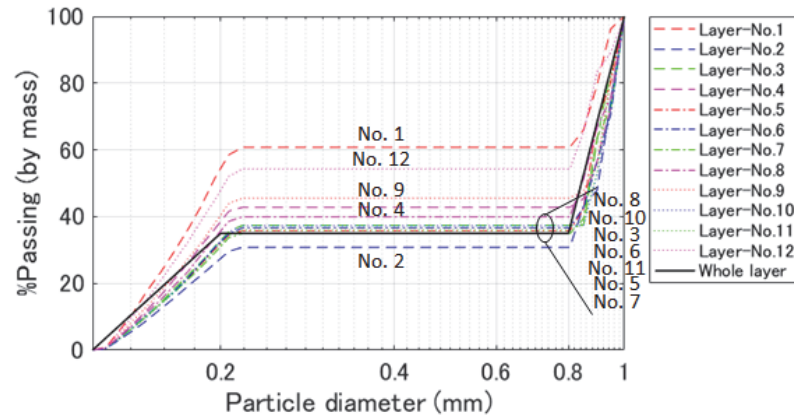


Figure 3.20 PSDs in each layer of large-dense sample with 35% fines

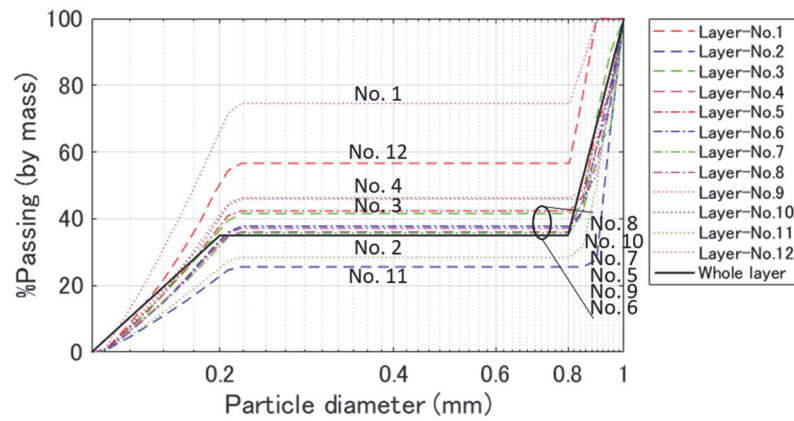


Figure 3.21 PSDs in each layer of pluviated large-loose sample with 35% fines

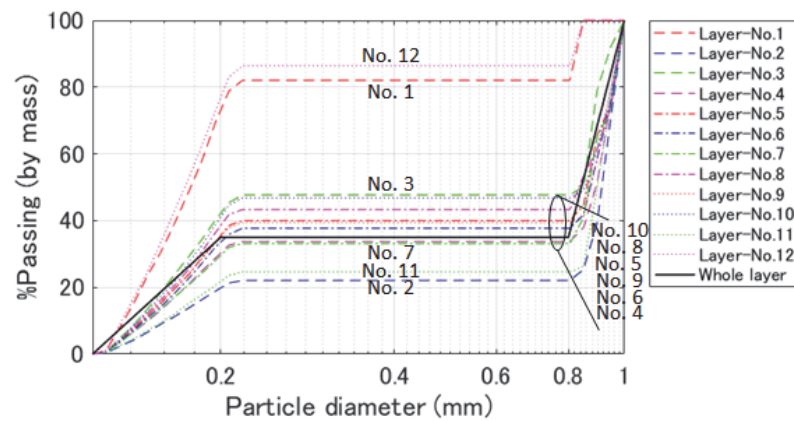


Figure 3.22 PSDs in each layer of pluviated large-dense sample with 35% fines

3.4.3. Stress reduction factor α

As shown in Equation 2.1, a key parameter to consider for these samples was α , the proportion of stress carried by the finer grains. To determine α , a MATLAB script was developed that takes as input data files listing the contact and particle data. To assess the effect of the boundaries, α was calculated using all the particles in the sample and using only particles within the central measurement sphere were considered to calculate α for this sub-volume. As shown in Figure 3.23, the particles that intersected the measurement sphere were identified so as to isolate this sub-set of particles. Then, the volume of a particle-measurement sphere intersection was calculated using Equation 3.5 as shown in Figure 3.24. Thus, the partial volumes of the intersected particles that were considered are as illustrated in Figure 3.25.

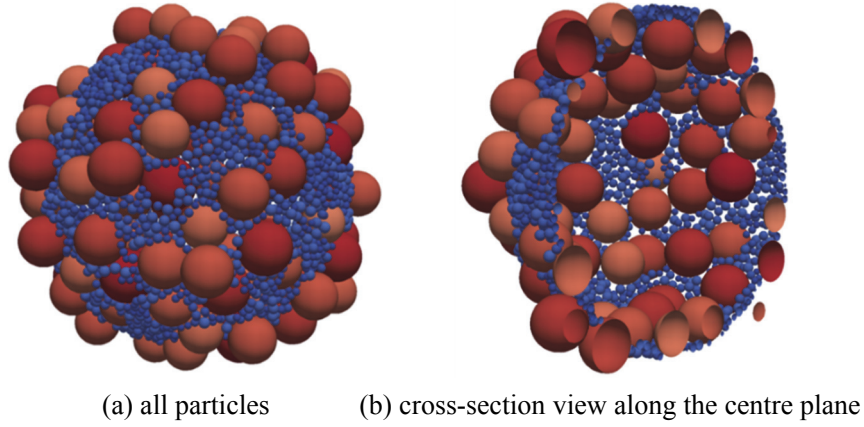


Figure 3.23 Particles on the intersection

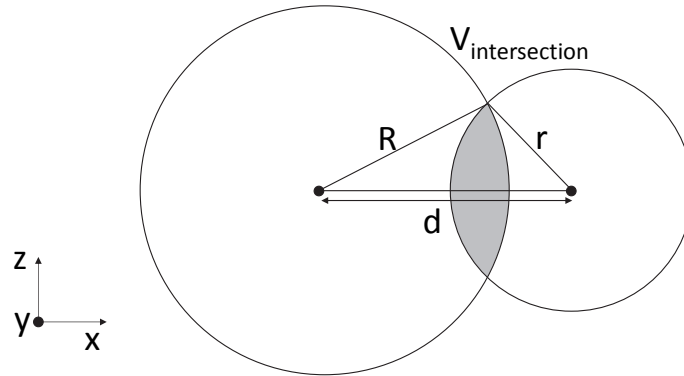


Figure 3.24 Schematic area of particle-measurement sphere intersection

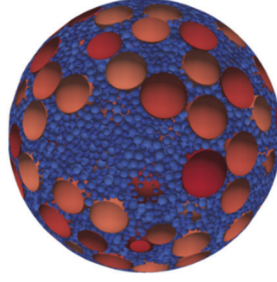


Figure 3.25 Particles including intersected particles within measurement sphere

$$V_{\text{intersection}} = \frac{\pi(R + r - d_{\text{cap}})^2(d_{\text{cap}}^2 + 2d_{\text{cap}}r - 3r^2 + 2d_{\text{cap}}R + 6rR - 3R^2)}{12d_{\text{cap}}} \quad 3.5$$

where $V_{\text{intersection}}$ = volume of sphere-sphere intersection (hatched area in Figure 3.24); R = radius of one particle; r = radius of the second particle; and d_{cap} = distance between centres of two spheres.

In Figure 3.26 and Figure 3.27, the distribution of mean normal stress is visualised on the four samples on an XZ-plane through the samples. Recall that the mean normal stress was given in Equation 2.4. Particles shaded in “red” transfer a significant amount of stress, whereas the “blue” particles transfer substantially less stress. For the loose samples in Figure 3.26, stress is preferentially transmitted by the coarse particles, when the centre of the figure is considered. As density increases, fines carry more stress as shown by comparing Figure 3.26 and Figure 3.27. In the loose samples, there is a higher proportion of low stress “blue” particles in the centre of the samples than for the dense samples in Figure 3.27. In the samples with 25% fines, a lot of low stress “blue” particles are seen between coarse particles. The heterogeneity in the smaller samples is very evident in Figure 3.26 and Figure 3.27. The small numbers of highly stressed particles in this small sample in Figure 3.26 (b) highlights the fact that this sample is too small to be considered an RVE.

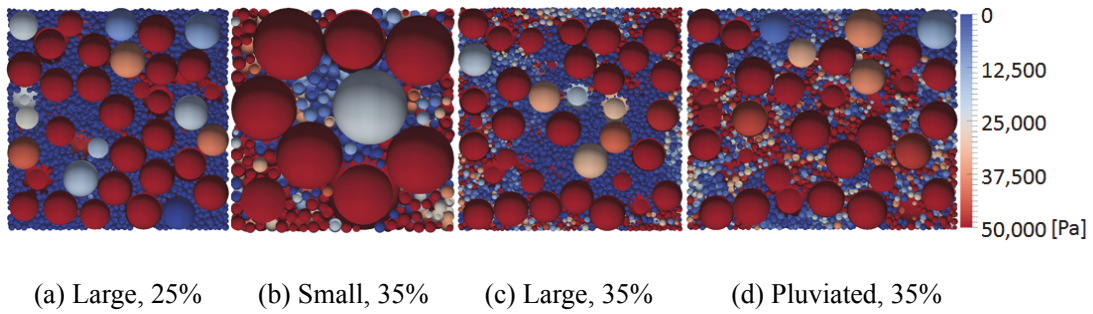


Figure 3.26 Distribution of mean normal stress in xz-plane with loose samples

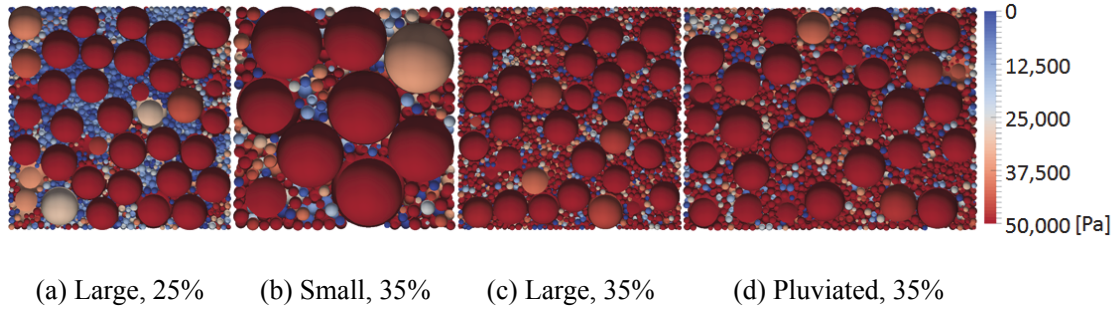


Figure 3.27 Distribution of mean normal stress in xz-plane with dense samples

Table 3.6 and Table 3.7 give the α values obtained from the whole sample and the measurement sphere, respectively. In these tables, there are four types of α : α, p' , α, σ_x , α, σ_y , and α, σ_z . α, p' is defined in terms of the mean normal stress, i.e. overall stress in the x, y, and z direction is taken into account ($\alpha, p' = \frac{\bar{\sigma}_{fine}}{\bar{\sigma}_{ij}}$). The other α values are calculated in terms of each direction: α, σ_x is the α in the x direction, α, σ_y in the y direction, and α, σ_z in the z direction. There are measureable differences when the α values from the different measurement volumes are compared. The values for the whole sample listed in Table 3.6 are significantly higher than the values for the measurement sphere only listed in Table 3.7. The ratio of α values calculated from the whole sample to α values obtained from the measurement sphere is shown in Table 3.9 as well. These data show the concentration of fines close to the boundary lead to an unrealistic increase in α values, excluding the large-loose sample with 25% fines. This shows that the observations of particle migration close to the boundaries in laboratory tests such as a triaxial test will not be representative of the material response.

The data presented in Table 3.6 and Table 3.7 indicate that the α values for the loose samples are smaller than those of the dense samples. The variation in α values with sample density (Table 3.6 and Table 3.7) confirms the observations (Table 3.8) of Shire et al. (2014) that this type of transitional fines content is sensitive to relative density, especially for the samples with 25% fines content. For the measurement sphere data in Table 3.7, the α values for the loose samples with 35% fines are roughly between 0.34 and 0.51 and decrease as the number of particles increases. The α values for the samples with 25% fines are between 0.10 and 0.44, and the α values for the samples with 35% fines are between 0.32 and 1.14 and increase as the number of particles increases. The results show that the α values for the samples with 25% are low because of the underfilled situation (Figure 2.4 (a)), whereas the α values for the samples with 35% are large because of the overfilled situation (Figure 2.4 (b)). Also, the α values for the pluviated samples are between 0.50 and 1.19. The variation in α values is similar to that for the

compressed samples. Here, only the α values in the measurement sphere for the loose sample with 25% fines are larger than those obtained from the whole sample. This is probably because the concentration of fine particles near the rigid walls is avoided due to the low number of fine particles as shown in Figure 3.26 (a).

As was the case for the porosity data in Table 3.4, the α values noted by Shire et al. (2014) are included on Table 3.7 (sample denoted Gap Med 25 and Gap Med 35). The results show that representative data can be obtained except the medium and dense sample with 25% fines, provided the boundary data are excluded. Plus, the representative data is quite insensitive to sample preparation method.

Table 3.6 α values calculated from throughout the whole sample including stress in both ends of layers ($\alpha, p' = \alpha$ values calculated from mean normal stress;

$\alpha, \sigma_x = \alpha$ values relating to x direction; $\alpha, \sigma_y = \alpha$ values relating to y direction; and $\alpha, \sigma_z = \alpha$ values relating to z direction)

Fines Direction	Large 25%			Small 35%			Medium 35%		Large 35%			Pluviated 35%		
	Loose	Medium	Dense	Loose	Medium	Dense	Loose	Medium	Loose	Medium	Dense	Loose	Medium	Dense
α_{whole}														
α, p'	0.106	0.186	0.432	0.791	0.918	0.952	0.687	0.976	0.641	0.991	1.178	0.636	0.965	1.183
α, σ_x	0.100	0.178	0.433	0.750	0.892	0.935	0.681	0.962	0.626	0.987	1.174	0.655	0.953	1.181
α, σ_y	0.112	0.189	0.423	0.845	0.951	0.972	0.695	0.973	0.635	0.994	1.179	0.654	0.991	1.194
α, σ_z	0.106	0.192	0.439	0.779	0.912	0.949	0.685	0.994	0.662	0.991	1.180	0.599	0.952	1.175

Table 3.7 α values calculated from particles within measurement sphere

Direction	Large 25%			Small 35%			Medium 35%		Large 35%			Pluviated 35%		
	Loose	Medium	Dense	Loose	Medium	Dense	Loose	Medium	Loose	Medium	Dense	Loose	Medium	Dense
$\alpha_{\text{meas, sphere}}$														
α, p'	0.141	0.139	0.304	0.506	0.694	0.740	0.430	0.830	0.341	0.836	1.128	0.552	0.947	1.171
α, σ_x	0.132	0.127	0.304	0.421	0.652	0.723	0.428	0.814	0.335	0.823	1.122	0.509	0.935	1.167
α, σ_y	0.143	0.144	0.288	0.616	0.757	0.802	0.437	0.839	0.327	0.850	1.119	0.606	0.974	1.188
α, σ_z	0.150	0.146	0.321	0.491	0.678	0.702	0.426	0.837	0.361	0.835	1.142	0.548	0.933	1.157

Table 3.8 α values (Shire et al., 2014)

Direction	Gap Med 25 25%			Gap Med 35 35%		
	Loose	Medium	Dense	Loose	Medium	Dense
$\alpha_{\text{meas,sphere}}$						
α, p'	0.18	0.33	0.76	0.34	0.86	1.15
α, σ_x	-		-	-	-	-
α, σ_y	-		-	-	-	-
α, σ_z	-		-	-	-	-

Table 3.9 Ratio of α from measurement sphere to that from the whole sample

Direction	Large 25%			Small 35%			Medium 35%		Large 35%			Pluviated 35%		
	Loose	Medium	Dense	Loose	Medium	Dense	Loose	Medium	Loose	Medium	Dense	Loose	Medium	Dense
$\alpha_{\text{meas,sphere}}$														
α, p'	1.33	0.75	0.70	0.64	0.76	0.78	0.63	0.85	0.53	0.84	0.96	0.87	0.98	0.99
α, σ_x	1.32	0.71	0.70	0.56	0.73	0.77	0.63	0.85	0.54	0.83	0.96	0.78	0.98	0.99
α, σ_y	1.28	0.76	0.68	0.73	0.80	0.83	0.63	0.86	0.51	0.86	0.95	0.93	0.98	1.00
α, σ_z	1.42	0.76	0.73	0.63	0.74	0.74	0.62	0.84	0.55	0.84	0.97	0.91	0.98	0.99

3.4.4. Fabric anisotropy

For the samples that were initially isotropically consolidated, prior to applying gravitational loading, any anisotropy must be due to the self-weight of the particles in the vertical z-direction after applying gravitational loading. The α values were calculated so as to get a feel as to whether such an anisotropy might influence susceptibility to internal erosion. However, the difference in stress was small. Here, the isotropic stress applied was $p' = 50$ kPa, and the additional stress in the vertical z-direction produced by applying gravity to 31,793 particles was approximately 116 Pa. Therefore, this stress is not capable of contributing the anisotropy. Despite this, particle rearrangement caused by gravity could still induce anisotropy. However, there is no systematic variation in α with direction. Referring to Table 3.7, the differences between α, σ_x and α, σ_y are similar to the differences between α, σ_z and both α, σ_x and α, σ_y . This observation holds for both compressed and pluviated samples. The heterogeneity was considered by comparing α values in the measurement sphere with the overall average α values. The loose samples are most heterogeneous.

In addition to stress anisotropy, contact anisotropy was also considered. Oda et al. (1985) showed that fabric can be quantified by using orientation data at the particle scale: unit contact normal vector, particle, void and branch vector. Satake (1982) defined a fabric tensor for quantifying fabric anisotropy as follows:

$$\Phi_{ij} = \frac{1}{N} \sum_{k=1}^N n_i^k n_j^k \quad 3.6$$

where Φ_{ij} = fabric tensor; N = total number of vectors; and n_i^k and n_j^k = k th unit orientation vector. This fabric tensor has been used in a number of DEM studies; for example, Thornton (2000) and Shire et al. (2012). Rothenburg & Bathurst (1989) suggested an equation including only two parameters where an ellipse is fitted by means of Fourier series, which was used by Barreto (2008). The equation of Rothenburg & Bathurst (1989) is shown in Equation 3.7:

$$E(\theta) = \frac{1}{2\pi} \{1 + a \cos 2(\theta - \theta_a)\} \quad 3.7$$

where a = magnitude of fabric anisotropy; and θ_a = direction of the fabric anisotropy or principal fabric.

Here, fabric anisotropy was quantified using unit contact normal vector. By using this concept proposed by Rothenburg & Bathurst (1989), both a and θ_a obtained from Equation 3.7 are indicated in Table 3.10. Referring to a in Table 3.10, each a in the XY, YZ, and YZ plane of the compressed sample has almost equal value, whereas the pluviated samples a smaller a in the XY plane in comparison with XZ and YZ plane, i.e. $a_{XY} < a_{XZ} = a_{YZ}$. This observation confirms that the pluviated samples are cross-anisotropic.

Table 3.10 Parameters of fabric tensor in each cross-section

Sample	Fines	a			θ_a (degrees)		
		XY-plane	XZ-plane	YZ-plane	XY-plane	XZ-plane	YZ-plane
Large-loose	25%	0.01	0.04	0.03	169	129	-126
Large-dense	25%	0.02	0.02	0.02	137	3	-22
Large-loose	35%	0.03	0.08	0.04	74	28	14
Large-dense	35%	0.02	0.03	0.01	15	17	42
Pluviated-loose	35%	0.02	0.13	0.11	-68	-27	0
Pluviated-dense	35%	0.02	0.08	0.07	-149	-22	-17

The orientation of contacts between particles is shown in Figure 3.28 to Figure 3.33. In each rose histogram, the bin length represents the number of contacts orientated within that bin's angular increment. 36 bins were considered to give 10-degree angular increments. The colour gradation stands for the magnitude of average contact force with a specific direction. Samples tend to have more contacts along the x, y and z directions. The directions with more contacts seem to have strong contact forces. However, no significant variation in a values is seen in Table 3.10. From the rose histograms, it is shown that the length of the histograms differs from sample to sample. The number of contacts between the particles in the loose and dense samples with 25% fines is almost same, whereas there are fewer contacts between the particles in the loose samples with 35% fines (Figure 3.30 and Figure 3.32) than in the dense samples with 35% fines (Figure 3.31 and Figure 3.33). This is related to the coordination number data shown in Table 3.2. As the number of particles becomes bigger and bigger, the data become more smooth. These figures imply that there is almost no fabric anisotropy in the compressed large samples due to gravity under $p' = 50$ kPa. The isotropic consolidation stress of $p' = 50$ kPa is relatively big in comparison with the impact of the gravity. However, the fabric anisotropy can be recognised in the pluviated samples, especially for the loose sample, as shown in Figure 3.32 and Figure 3.33.

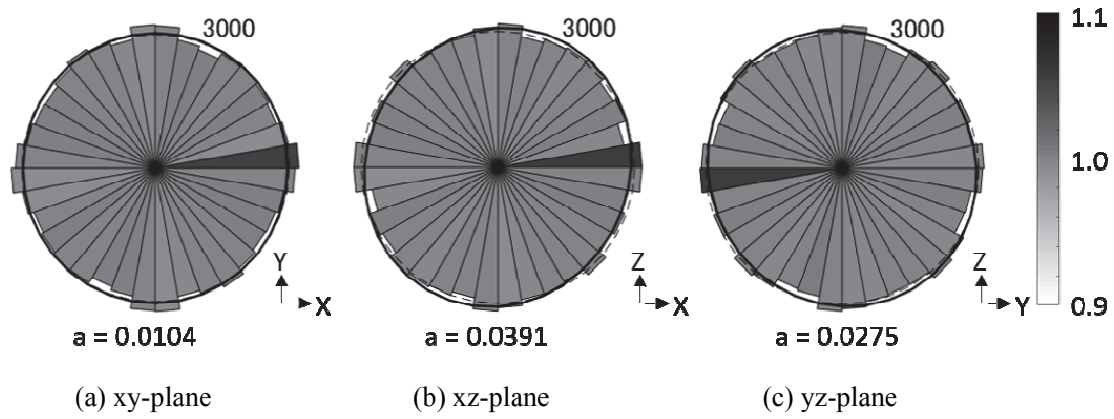


Figure 3.28 Rose histograms of fabric anisotropy for large-loose sample with 25% fines

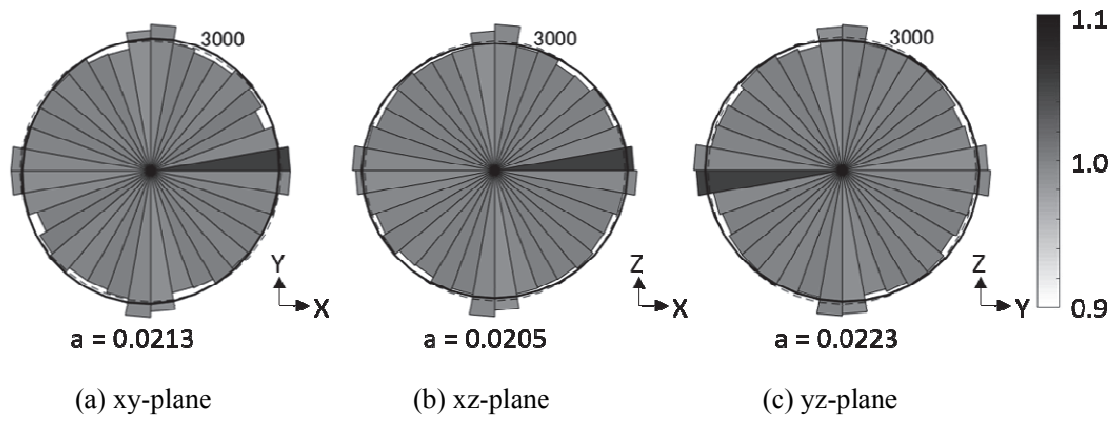


Figure 3.29 Rose histograms of fabric anisotropy for large-dense sample with 25% fines

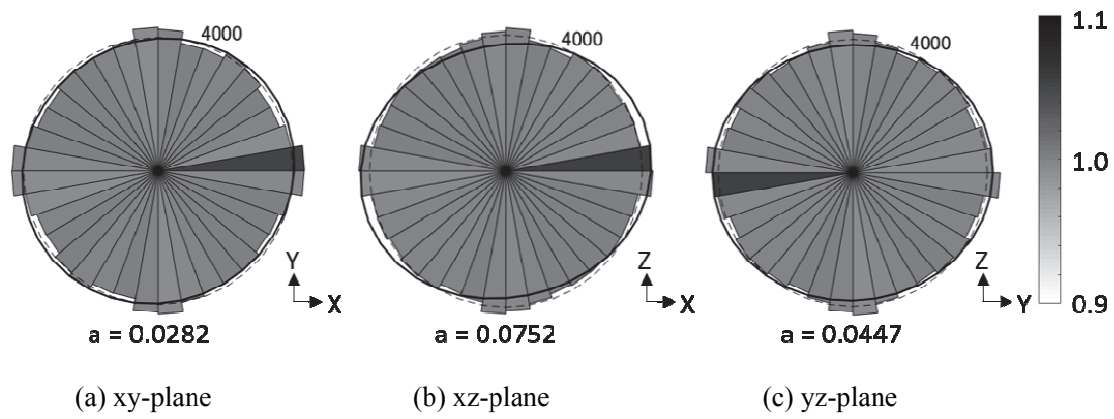


Figure 3.30 Rose histograms of fabric anisotropy for large-loose sample with 35% fines

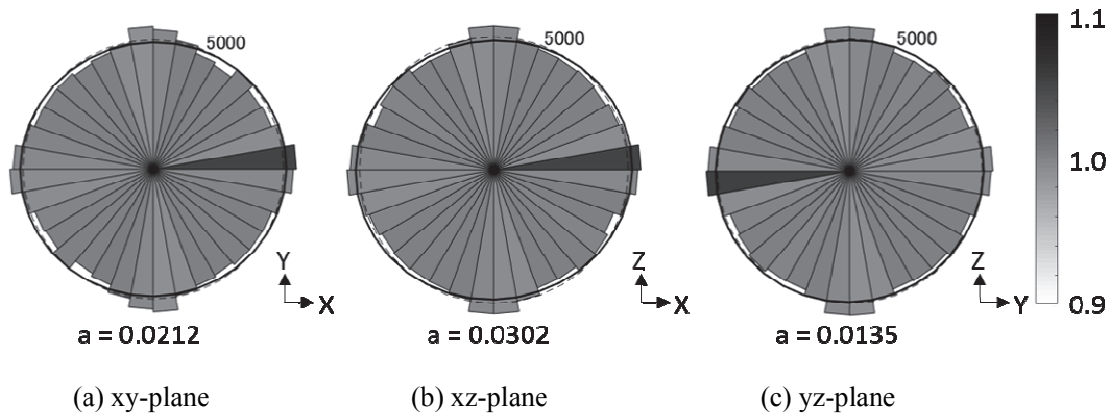


Figure 3.31 Rose histograms of fabric anisotropy for large-dense sample with 35% fines

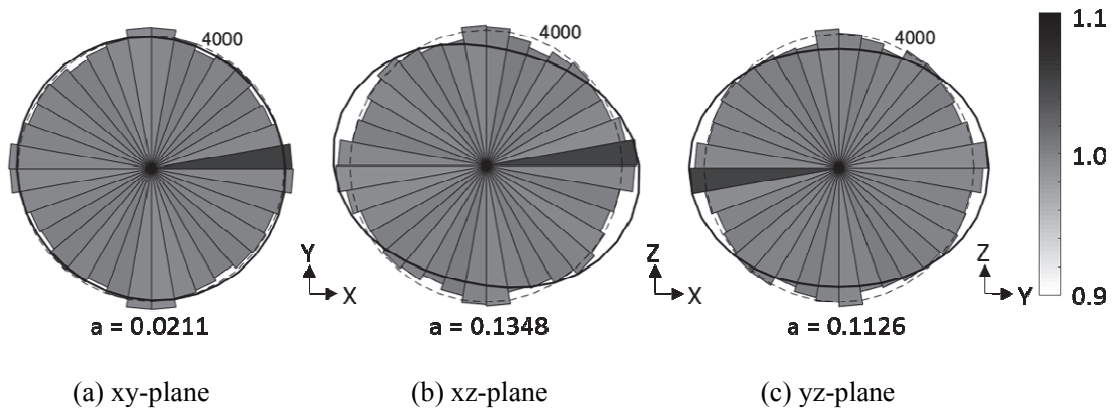


Figure 3.32 Rose histograms of fabric anisotropy for pluviated loose sample with 35% fines

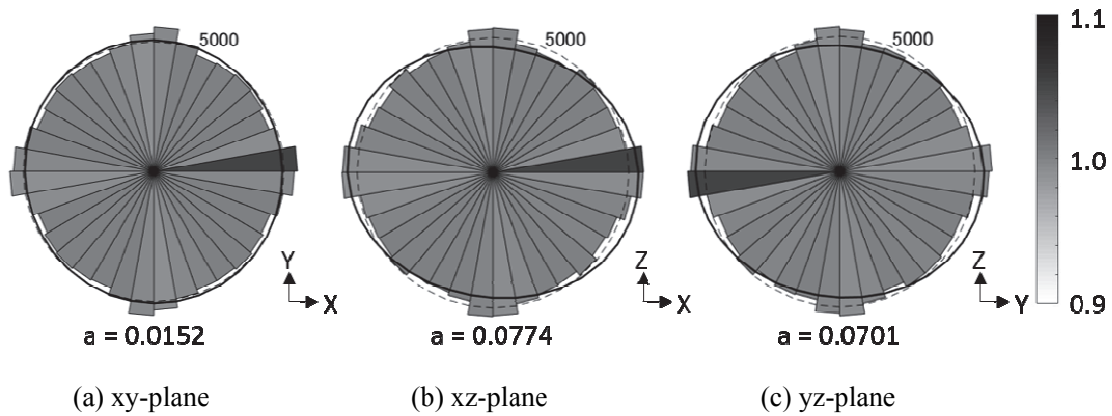


Figure 3.33 Rose histograms of fabric anisotropy for pluviated dense sample with 35% fines

Chapter 4. PARTICLE-FLUID INTERACTION USING A COUPLED DEM-CFD PROGRAM

4.1. Introduction

The overall objective of this study is to apply particle-scale analysis of seepage flow through a packed particle assembly under a specific confining pressure and hydraulic gradient to gain insight into internal instability. This chapter introduces the coupled DEM-CFD (Computational fluid dynamics) scheme used. Section 4.2 describes the general coupling approach adopted. Section 4.3 outlines how the commercial DEM-CFD coupled codes used here (PFC3D-CCFD) work. Section 4.4 discusses refinements that were made to the two codes by the software companies involved, which was based on results that emerged from this study. Finally, Section 4.5 presents some validation exercises.

4.2. Coarse grid approach to coupled DEM simulations

Ideally a coupled particle-fluid interaction model would be able to capture the complexity, i.e. the fluid velocity and drag forces would be resolved at a scale significantly smaller than the voids and the particles. Models which are able to do this, e.g. the mirroring immersed boundary method (Mark & van Wachem, 2008), require prohibitively large computational capacity for coupling with a large number of DEM particles. For this reason the coarse-grid fluid model is adopted here. As the initial packing porosity is relatively homogeneous (Section 3.4.2), the drag forces acting on the particles at the point of initiation should be relatively well modelled by the coarse grid method as shown in Figure 4.1 (a). However, as the fluid is not resolved at a scale smaller than an individual void, the model will not be able to capture some aspects of internal instability; for example, localised flow when erosion occurs locally within a single void (Figure 4.1 (b)). For this reason, code is to be used to study initial particle detachment due to seepage only. Progression to full erosion would require the use of a more sophisticated model, such as that developed by (Chareyre et al., 2012).

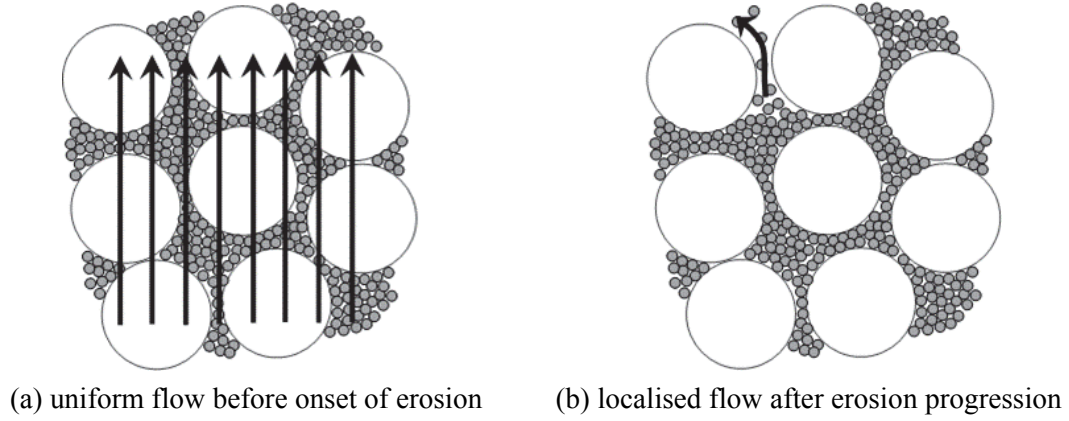


Figure 4.1 Schematic drawings of different water flow

4.2.1. Averaged Navier-Stokes equations

Use of the averaged Navier-Stokes equations approach is the most common way to carry out coupled particle-fluid analyses with DEM. This approach has previously been used in geomechanics research by Zeghal & El Shamy (2008) and Climent et al. (2014). The approach was originally proposed by Tsuji et al. (1993) who were interested in simulating fluidised beds for chemical engineering applications. Tsuji et al. (1993) considered Anderson & Jackson (1967) who proposed that the continuity and momentum equations can be calculated by using local average values, so that averaged Navier-Stokes equations describe the fluid flow. Overviews of this approach are given in Tsuji et al. (1993), Xu & Yu (1997) and Kafui et al. (2002). In the method, a regular grid is overlaid on the system of particles considered in the DEM simulation. The size of a fluid grid cell is larger than the particle size as illustrated in Figure 4.2. Water flow between individual pores is not modelled, rather an average value is determined in each cell. As shown in Figure 4.2, one fluid cell length typically exceeds five average particle diameters. The averaged continuity equation is given by Kafui et al. (2002) as follows:

$$\frac{\partial(n\rho_f)}{\partial t} + \nabla(n\rho_f\vec{v}_f) = 0 \quad 4.1$$

where ρ_f is the fluid density; $\vec{v}_f$ is the fluid velocity; t is time; and n is porosity as before. Assuming that water is Newtonian and incompressible, the averaged momentum equation is given as follows:

$$\frac{\partial n\rho_f\vec{v}_f}{\partial t} + \nabla(n\rho_f\vec{v}_f\vec{v}_f) = -n\nabla P + \nabla n\vec{\tau}_f + n\rho_f\vec{g} - \vec{F}_{fluid} \quad 4.2$$

$$\overrightarrow{F_{fluid}} = \frac{n_c}{\Delta V_c} n \overrightarrow{F_{drag}} \quad 4.3$$

where P is the fluid pressure; $\overrightarrow{\tau_f}$ is the viscous stress tensor; $\vec{g}$ is acceleration due to gravity; $\overrightarrow{F_{fluid}}$ is the particle-fluid interaction force per unit volume; n_c is the number of particles in a fluid cell; ΔV_c is volume of the fluid cell; and $\overrightarrow{F_{drag}}$ is the drag force per unit volume. The two terms on the left side of Equation 4.2 are the inertia force. The terms on the right side consider pressure, viscosity, buoyancy and interaction force including drag force respectively. Particular attention must be given to the calculation of $\overrightarrow{F_{fluid}}$.

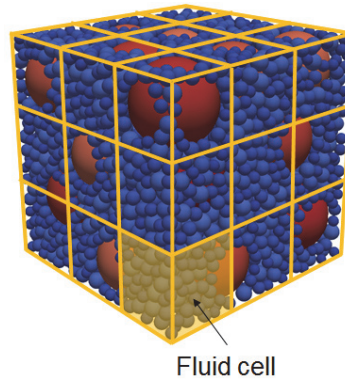


Figure 4.2 Schematic of particles and fluid cells

4.2.2. Particle phase

When a soil particle is submerged in a fluid as illustrated in Figure 4.3, the different types of interaction forces acting on it include a gravitational force and a particle-fluid interaction force comprising a buoyant force, a drag force and a pressure gradient force. The particle motion is governed by the Newton's second law:

$$m \frac{dv_p}{dt} = mg + F_{fluid} = F \quad 4.4$$

where m is the particle mass; v_p is the particle velocity; g is acceleration due to gravity; F_{fluid} is the particle-fluid interaction force; and F is the total force. The particle-fluid interaction force can be partitioned into hydrostatic and hydrodynamic forces. The hydrostatic force is linked to the buoyant force, whereas the hydrodynamic force is based on the drag force, which is the dominant interaction force (Zhu et al., 2007), and the pressure gradient force. The drag force is discussed further in Section 4.2.3 below.

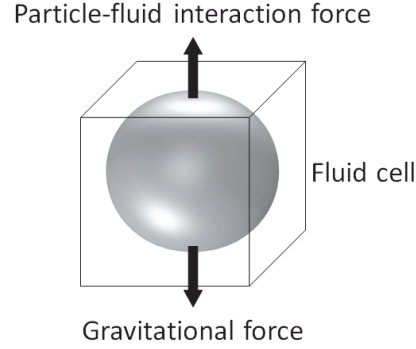


Figure 4.3 Forces exerted on a submerged soil particle

With regard to the averaged Navier-Stokes equations including particle-fluid interaction forces, two approaches have been proposed to quantify the force acting on the particles. These were termed Model A and Model B by Gidaspow (1994). Model A is based on a pressure gradient force model and assumes that the particle-fluid interaction force is divided between the particles and the fluid. In this case, the empirical drag correlation accounts for pressure gradient force as shown in Equation 4.5. On the other hand, the pressure gradient force acts only on the fluid in Model B, which is based on a fluid density-based buoyancy. In this model, the empirical drag correlation does not account for pressure gradient force as shown in Equations 4.6.

$$\text{Model A} \quad F_{fluid} = nF_{drag} \quad 4.5$$

$$\text{Model B} \quad F_{fluid} = nF_{drag} - \nabla P V_p \quad 4.6$$

where V_p is the volume of a particle. Model A was used for simulation of fluidised beds (an application of interest to chemical engineers) by Tsuji et al. (1993). In geotechnical engineering, Model A was used for simulation of seepage flow through saturated particle assembly by Suzuki et al. (2007) and Chen et al. (2011), whereas Model B was used for the analysis of liquefaction by Zeghal & El Shamy (2004) and Zeghal & El Shamy (2008) and has been adopted in the PFC-CCFD software used here (Section 4.3). Both Models A and B were considered by Bouillard et al. (1989) and Kafui et al. (2002), and they clarified the difference between Model A and B. Bouillard et al. (1989) showed that no significant differences in bubble shapes, sizes, or bubbling frequencies between these models. In the work of Kafui et al. (2002), although a better agreement with pressure drop calculated by the Ergun equation can be seen for Model A than for Model B, the difference is just 10%, which is discussed in the following section.

4.2.3. Drag force

The drag force is strongly related to seepage flow velocity. The drag force can be estimated using empirical equations including those originally developed by Ergun (1952) and Di Felice (1994). The Ergun equation (Ergun, 1952) was developed from experiments that measured the pressure drop when water flow flowed through fixed beds of granular materials having uniform geometric shapes. This equation is given by:

$$F_{drag} = 150 \frac{\pi d \mu_f (1-n)}{6n^2} v_r + 1.75 \frac{\pi d^2 \rho_f}{6n} v_r^2. \quad 4.7$$

where d is the particle diameter; μ_f is the fluid viscosity; and v_r is the relative velocity between fluid and particles. On the right side of Equation 4.7, the first term is the viscous term, and second term is the inertia term. The viscous term is based on the Kozeny-Carman equation that is commonly used to predict the pressure drop of a fluid flowing through fixed beds of solids and is dominant at lower water flow velocities, which is typically the case in geotechnical engineering. The Ergun equation is typically used for materials with porosity of $n < 0.8$ according to Kafui et al. (2002). For higher porosities, the equation proposed by Wen & Yu (1966) is more appropriate. The Ergun equation has been applied to geotechnical research in the work of Zeghal & El Shamy (2004), Suzuki et al. (2007), Cheung (2010) and Chen et al. (2011).

The Di Felice equation (Di Felice, 1994) was derived from experimental data for pressure loss through both fixed beds and fluidised beds of granular materials. This equation is modified to take account of neighbouring particles and expressed as follows:

$$F_{drag} = C_D \frac{\rho_f v_f \pi d^2}{2} |v_f| n^{-x} \quad 4.8$$

where $C_D = \left(0.63 + \frac{4.8}{Re^{0.5}}\right)^2$ is the drag coefficient for a single spherical particle; $Re = \frac{2r \rho_f v_f}{\mu_f}$

is the particle Reynolds number; and $x = 3.7 - 0.65 \exp\left(-\frac{(1.5 - \log_{10} Re)^2}{2}\right)$ is the voidage function, which accounts for the influence of neighbouring particles on the drag coefficient. The Di Felice equation has been implemented in the PFC3D-CCFD code used here and in published DEM-CFD research, e.g. Kafui et al. (2002) and Climent et al. (2014). This equation is considered to be valid for a wide range of porosities and Reynolds numbers.

In geotechnical engineering, a uniform sand typically has a porosity in the range between 0.3 and 0.5, and a well graded sand typically has a porosity between 0.2 and 0.45, whereas the porosity of a silty sandy gravel can be less than 0.12 (Mitchel & Soga, 2005). On the other hand, the experiments carried out in the work of Ergun are based on materials with $0.4 < n < 0.65$, which would be considered a low density in geotechnical engineering. The Di Felice equation was developed for materials with $0.4 < n < 1.0$. To make the difference between these equations clear, the drag force, varying as a function of porosity, in the case of the water velocity of 0.01 m/s and 0.005 m/s is drawn in Figure 4.4. In this example, the particle size is set to be 1 mm in diameter. For the same water velocity of 0.005 m/s, the magnitude of the drag force that is calculated by the Di Felice equation is smaller than that calculated by the Ergun equation beyond the porosity of 0.38, whereas the drag force calculated by the Di Felice equation is larger than that calculated by the Ergun equation under the porosity of 0.38. For the same water velocity of 0.01 m/s, the magnitude of the drag force calculated by the Di Felice equation is larger than that calculated by the Ergun equation over a wide range of porosities.

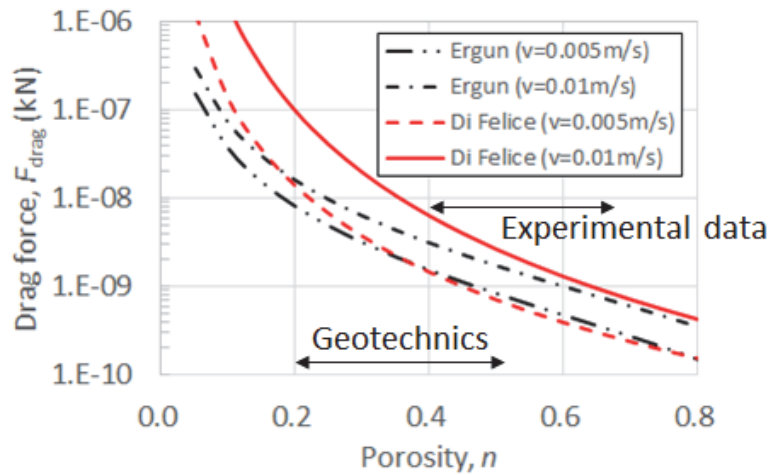


Figure 4.4 Comparison with Ergun and Di Felice equation with different flow velocities

4.3. Overview of software used

In this research, the commercial DEM-CFD code of PFC3D-CCFD is used. The discrete element method (DEM) software PFC3D is used to model the particle phase and the computational fluid dynamics (CFD) software CCFD is used to model the fluid. The PFC3D software is developed by Itasca Consulting Group, Inc., while the CCFD add-on is developed by ITOCHU Techno-Solutions Corporation (CTC). In the current study, the PFC3D version 5.00.25 (Itasca Consulting Group, 2016) was used. The CCFD add-on is a separate piece of software, which was purchased from CTC, and version 2.0.4rc3 was used. Note that most CCFD commands were revised, for the version 5.00.25 of PFC3D was released. Accordingly, input

files created by version 5.00.24 and older were not run in the latest version of 5.00.25. In addition to these computer programs, a pre- and post- processor for numerical simulation, which is called GiD version 8.0.9, was used. This is developed by the International Centre for Numerical Methods in Engineering. Note that there is a later version of GiD, however only the version 8.0.9 can be used with the PFC3D-CCFD program used here. It has been designed for geometrical modelling, creating meshes, data transfer to numerical analysis programs, as well as the visualization of numerical results. The nature of this approach to coupling, where the two main codes (PFC and CCFD) were developed by two separate companies, one based in the USA and the second based in Japan, posed a particular challenge to delivery of the research described here.

The coupled simulation process is illustrated schematically in Figure 4.5. In practice, the PFC3D time step is smaller than the CCFD time step, i.e. several cycles of the PFC3D are needed for each CCFD cycle, so that the coupled information is exchanged each fluid cycle. For the analyses presented here, there were about 1,000 DEM cycles for each fluid cycle.



Figure 4.5 Process of conducting DEM-CFD program

4.3.1. Boundary conditions

In PFC3D, there are four types of boundary conditions: stop, reflect, destroy, and periodic. The stop condition imposes the constraint that the velocity and spin (rotational velocity) of particles are set to zero if the centroid of each particle falls outside the model domain. The reflect condition reverses the velocity direction and does not change the spin. The destroy condition means that a particle will be deleted if its centroid falls outside the model domain. When the periodic condition is used, if a particle centroid falls outside the periodic domain, it is transferred to the opposite side of the domain. Although use of periodic boundaries condition would improve the spatial homogeneity of particle assembly, the stop condition is applied since the periodic boundary condition cannot be used in the CCFD add-on.

In the CCFD add-on, two types of boundary conditions can be applied: free slip and no slip. In the system considered here, the direction of water flow is upward. To achieve this condition, a free slip boundary condition is applied to the lateral walls and, for example, formulated as Equations 4.9 and 4.10. A free slip boundary condition means that normal velocity component

on the boundary is zero and two other components do not change across the boundary as shown in Figure 4.6.

$$v_{x,y} = 0 \quad 4.9$$

$$\frac{\partial v_y}{\partial x} = \frac{\partial v_z}{\partial x} = \frac{\partial v_x}{\partial y} = \frac{\partial v_z}{\partial y} = 0 \quad 4.10$$

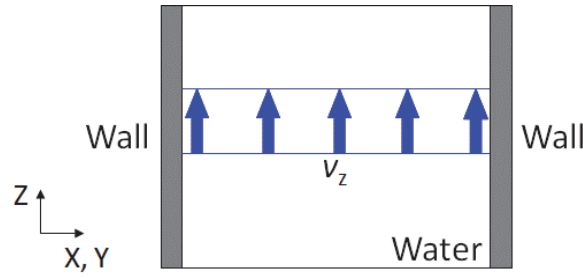


Figure 4.6 Free slip boundary condition

On the other hand, a no slip boundary condition requires all velocity components on the boundary to be zero (Equation 4.11) as shown in Figure 4.7.

$$v_x = v_y = v_z = 0 \quad 4.11$$

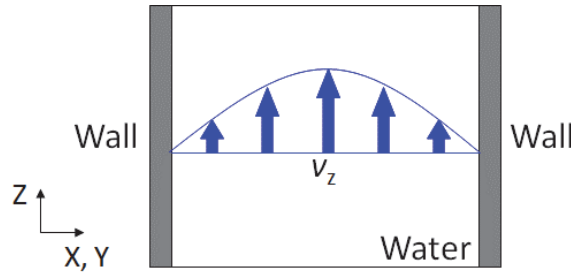


Figure 4.7 No slip boundary condition

4.3.2. Time integration

As shown in Figure 4.5, PFC3D and CCFD are regularly exchanging data. There are three types of time steps: a time step for a particle (DEM simulation time step), a time step for fluid and a time step for exchanging data as mentioned in Section 4.3. The time step for the fluid phase must be selected to achieve numerical stability. In CCFD, numerical stability is achieved by considering the Courant number (C), which is defined as:

$$C = \frac{v_f \Delta t_f}{\Delta l} \quad 4.12$$

where v_f is the fluid velocity; Δt_f is the time step for the fluid; and Δl is one fluid cell length. In the simulations considered here, the fluid cell length (Δl) is constant, thus the Δt_f can significantly affect C . C shows how much information traverses a fluid cell in a fluid calculation time step. If $C \leq 1$, information cannot move through an entire fluid cell in a single time step, whereas information can propagate through more than one fluid cell at each time step if $C > 1$. This means that a fluid cell does not have time to interpret what is physically happening by next time step for fluid, resulting in numerical oscillations. Smaller C values increase numerical stability with an increment in simulation time. In the study, C value was set to have 0.2 as a maximum value, and CCFD then calculated whether C value is always smaller than 0.2 using Δt_f given in the simulation. If C value is greater than 0.2, Δt_f is automatically recalculated to obtain an adequate C value.

CCFD adopts the Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) algorithm for incompressible fluid to solve the averaged Navier-Stokes equations. This algorithm was originally developed by Patanker (1980). In the CCFD program, which is based on the finite volume method (FVM), the averaged Navier-Stokes equations in terms of continuity (Equation 4.1) and momentum (Equation 4.2) are used. In the SIMPLE method, the fluid velocity is determined by using the momentum equation, and then a pressure estimate is obtained by using the continuity equation although continuity is not satisfied yet. This pressure estimate is substituted into the momentum equation in order to calculate fluid velocity. After repeating of this in an iterative process calculation, accurate fluid velocities and pressures can be obtained, which satisfy the continuity equation. According to a telephone interview to Mr. Akihiro Satoh, who is in charge of developing the CCFD code, at CTC on 20th November 2015, CCFD is based on collocated grids (Figure 4.8 (a)), i.e. fluid velocity and pressure are calculated in the centre of each fluid cell, so that simulation time can be shortened in comparison with staggered grids (Figure 4.8 (b)). The SIMPLE method is only applicable with staggered grids since velocity should be calculated on the cell boundaries using the continuity equation. Therefore, the Rhie-Chow Interpolation method (Rhie & Chow, 1983) is used to interpolate velocities to the cell boundaries even though the fluid cells are based on collocated grids as shown in Figure 4.9. Note that collocated grids are more susceptible to hourglass effects than staggered grids, i.e. numerical oscillation must be considered (further details will be given in Section 4.4.5).

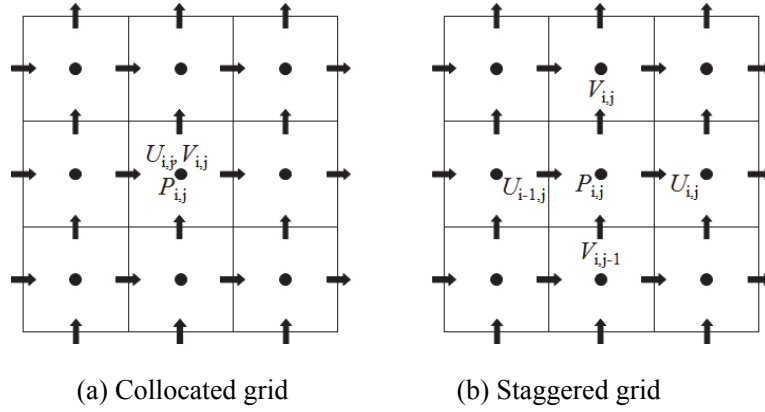


Figure 4.8 Different types of grids

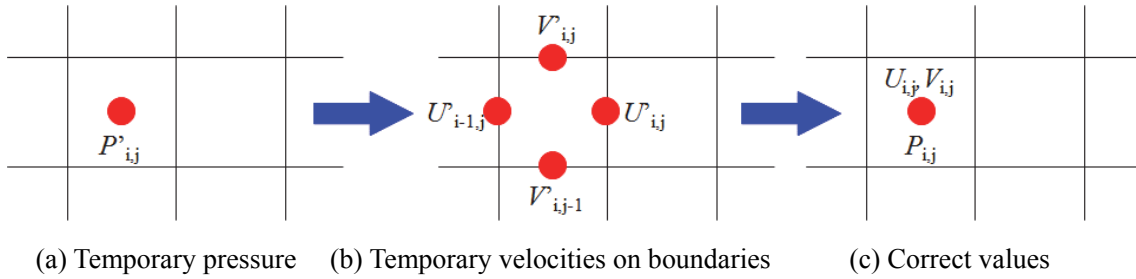


Figure 4.9 Rhie-Chow interpolation method

4.4. Code refinements

In the first 15 months of this research study, a number of limitations of the PFC3D-CCFD coupled simulation system were identified. These shortcomings were communicated to Itasca and CTC, and the PFC3D-CCFD code was modified accordingly. This process was time consuming and limited the overall research scope. Each of the resultant modifications is described briefly here.

4.4.1. Contact force error

For the application of interest here, the contact force between particles subject to gravity loading is an important output parameter. A simple initial simulation was considered as shown in Figure 4.10, i.e. single ball in a cubic column. A review of the results from this simulation revealed that an error in PFC3D version 5.00.17 was causing the particle-fluid force to be accounted for twice during the data exchange process of the CCFD software as illustrated in Figure 4.10. This error was fixed after the PFC3D version 5.00.18 was released on 29th April 2015.

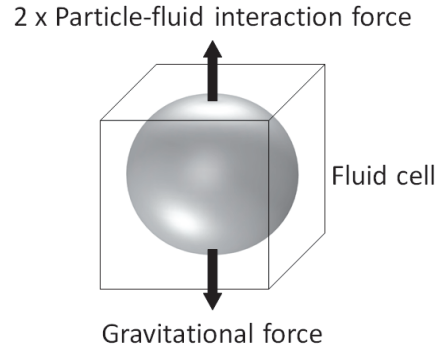


Figure 4.10 Calculated gravity force before code modification

4.4.2. Sensitivity to normal force

One approach to simulation considered here included vertical (lateral) periodic boundaries with rigid walls at the top and bottom. Preliminary simulations revealed that the normal force was unstable and suddenly became zero when a spherical particle touched the edge of periodic domains as shown in Figure 4.11. This bug was caused by the wall resolution logic. In PFC, a wall is a manifold, i.e. it is an orientable and edge-connected surface composed of facets in 2D that are linear segments according to the PFC manual (Itasca Consulting Group, 2007). If a wall is created as a single wall that spans the entire periodic domain boundary as shown in Figure 4.12 (a), all of the contact state information will be lost. To avoid this bug under periodic boundary conditions, a wall should be created as the combination of a single wall and facets, which are used for extending an initial wall to make arbitrary shapes, as shown in Figure 4.12 (b). This approach was developed by Matthew Purvance at Itasca on 8th May 2015. Furthermore, it is important to extend the domain of PFC3D beyond the PFC3D walls and the CCFD domain.

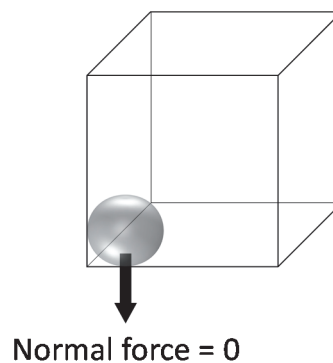


Figure 4.11 Ball touching edge of periodic boundaries

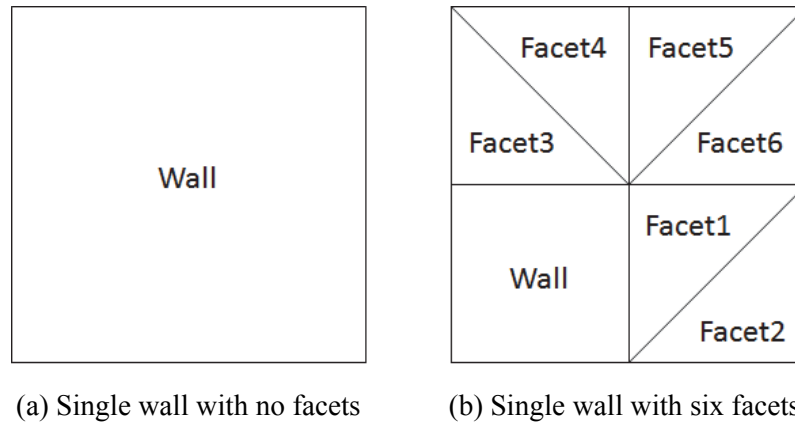


Figure 4.12 Method to create a single wall

4.4.3. Insufficient precision

In a parametric study to consider the effect of time increments on results, it was realised that some simulations were instantaneously terminated. The problem was caused by the numeric precision. Specifically, values after five decimal places, which were used in the time increment for data exchange between PFC3D and CCFD program, were totally ignored as the time increment is written as “15.5f” in FORTRAN format in the CCFD code. For example, a time step of $1\text{E-}6$ (six decimal points) was ignored as it was recognised as a value of 0; therefore, simulations did not work properly. After an update file, which was developed by Mr. Akihiro Satoh at CTC on 13th October 2015, was applied to the existing DEM-CFD program, this problem was fixed. After the problem was fixed, the effect of time increments on results was investigated as explained in Section 4.5.1.

4.4.4. Perturbation

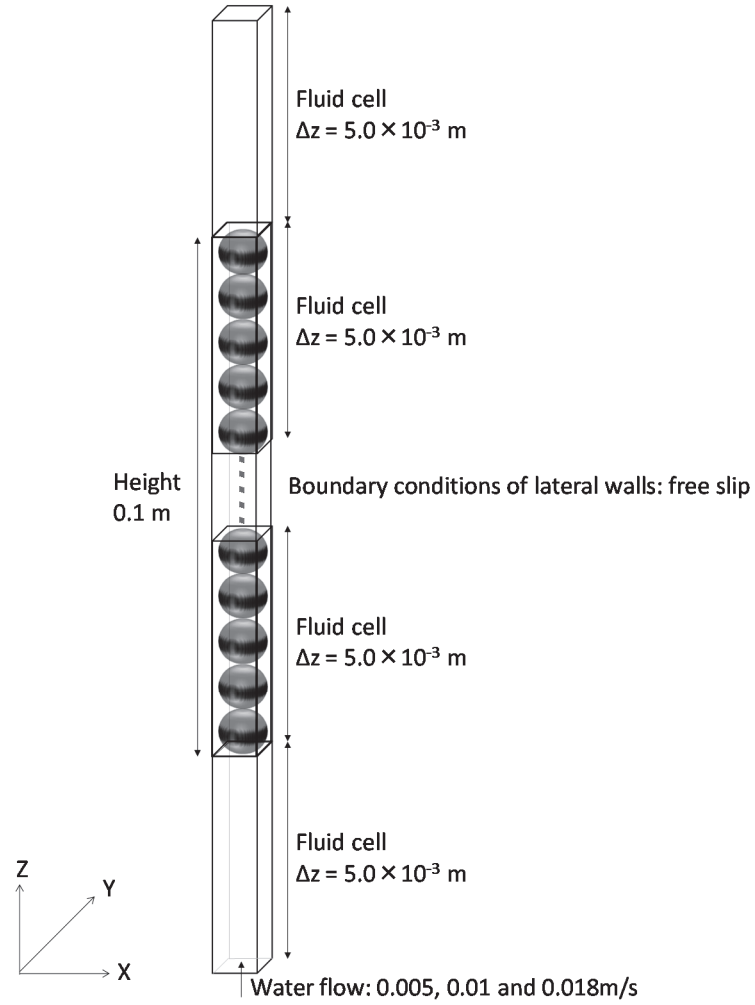
In developing the model, it was important to be able to apply water flow during a simulation since the water flow should be applied after all the particles have settled down under gravity and buoyancy forces. To enable application of the water flow at any arbitrary time, PFC3D allows users to generate a save file to resume simulation, i.e. to restart a previous simulation. A save file is used to save the current state of the system and includes all information such as boundary conditions, ball information and the ball physical properties. A save file is approximately proportional to the size of the model. For instance, a model consisting of 500,000 balls with 3,500,000 contacts results in a save file of roughly 3 GB. The fluid cells were generated in CCFD software, and then particle assembly is placed within the fluid cells in PFC3D software using a save file. After all particles were placed in the fluid cells, the drag forces were calculated. There are two ways to apply arbitrary water flow after each particle under hydrostatic conditions: using a restart command or with a user defined function, which is based on the computer language

of C++. Initially, the restart command, which is called “CCFD restart”, was used in the PFC3D-CCFD program; however, this method was not satisfactory even when the water flow applied was zero. The sample configuration is based on the work of Suzuki et al. (2007), which is illustrated in Figure 4.13. This problem configuration is discussed further in Section 4.5.2 below. As shown in Figure 4.14, it is clear from this figure that non-physical oscillations in top particle position in the z direction were observed even when the fluid flow of 0 m/s was activated using the restart command. Therefore, a user defined function, which was based on C++, was created instead of using the restart command. The advantage of using the user defined function is that the water flow can be applied without restarting simulations, i.e. it can be applied in the process of simulations. After this function was compiled with Visual Basic Studio 2015 (the product of Microsoft), the simulation could be implemented without a perturbation. The example code of applying water flow during simulation, which was developed by Mr. Akihiro Satoh at CTC on 16th June 2015, is shown as follows:

```
DLL_BOUND_DATA( USER_VEL ) // Specify the name of a parameter
{
    double time = data.getTime(); // Obtain CCFD time
    if( time > EQUILI_TIME ) { // Specify when fluid velocity is applied
        return VELOCITY; // Specify fluid velocity used
    } else {
        return VELOCITY; // Apply designated fluid velocity
    }
}
```

Note that *USER_VEL*, *EQUILI_TIME* and *VELOCITY* need to be specified by users.

Boundary condition of top wall: fixed pressure = 0Pa



Boundary condition of bottom wall: fixed velocity of water flow

Figure 4.13 Column configuration (bottom ball: No. 1, top ball: No. 100, after Suzuki et al., 2007)

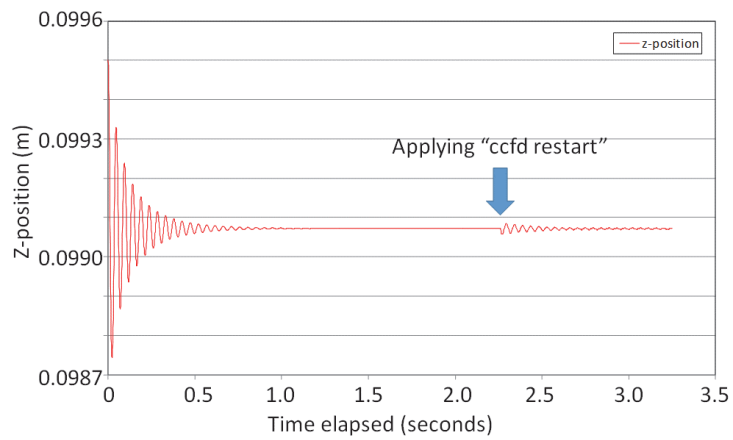


Figure 4.14 Perturbation in top particle z-position after using the restart command

4.4.5. Continuity

Each fluid cell must satisfy the continuity considerations, i.e. the inlet water flow must be the same as the outlet water flow. When the initial version of the CCFD add-on was used, it was realised that continuity was breached in some simple cases. The sample configuration used to make the observations is based on the work of Suzuki et al. (2007), which is illustrated in Figure 4.13. This problem configuration is discussed further in Section 4.5.2 below. A fluid velocity of 0.005 m/s was applied from the bottom of a square column. As shown in Figure 4.15 (a), considering three time intervals after application of the fluid flow, the fluid velocity at the bottom of the square column exceeded the applied velocity of 0.005 m/s, and average velocity throughout the column exceeded the applied velocity of 0.005 m/s. The fluid velocity at each fluid cell did not vary with simulation time, i.e. the fluid velocity in the vertical direction at a given elevation was the same after 1, 5, and 15 seconds. After this issue was identified, Itasca and CTC updated the CCFD add-on three times. With the use of the latest version of CCFD add-on released on 5th January 2016, continuity was achieved when the results converged after 15 seconds. After convergence, the fluid velocity obtained at each cell achieved the target fluid velocity of 0.005 m/s. However, relatively large numerical oscillations were found at smaller times, e.g. 1 second as shown here. These oscillations are problematic as they could generate non-physical drag forces since drag force is strongly linked to fluid velocity as indicated in Equations 4.7 and 4.8. For example, the discrepancy of drag force between 0.1 and 4 seconds is almost 30% as illustrated in Figure 4.16. In order to avoid the numerical oscillation, all balls were specified to be fixed in space until the fluid phase converged to avoid non-physical movement of particles.

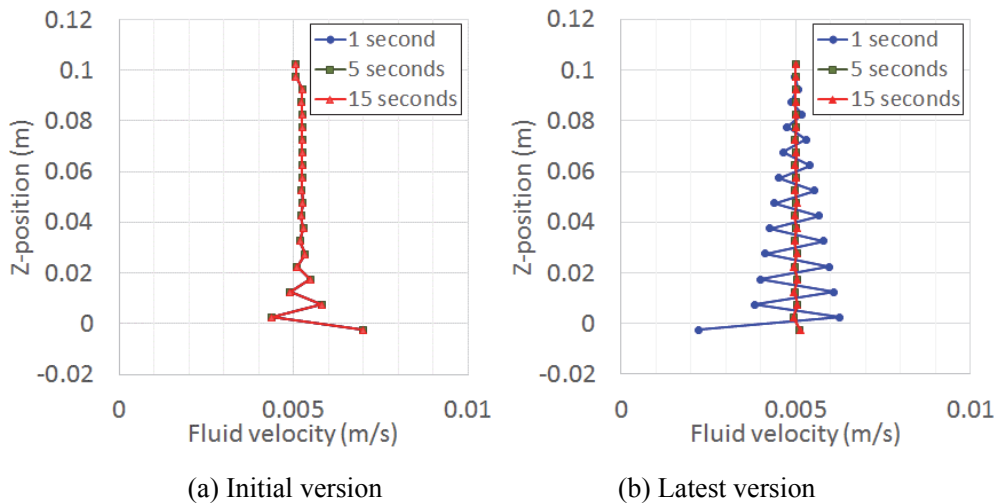


Figure 4.15 Fluid velocity at each fluid cell obtained by different CCFD add-on implemented

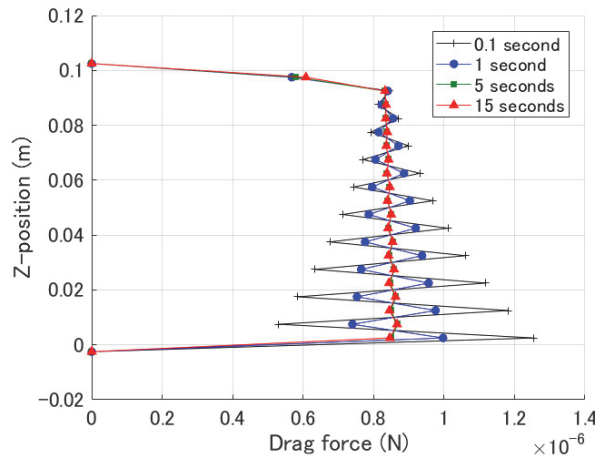


Figure 4.16 Drag force exerted on each ball

4.5. Validation exercises

Even though the software used was commercially developed, validation was important to show that this code was correctly implemented and to show that it was correctly used, prior to applying the system of codes in original research.

4.5.1. Single particle system

The first verification considers a spherical particle falling under gravity in a static fluid with a high Reynolds number (Figure 4.17). This example was chosen as it is simple and an analytical solution to the final terminal velocity can be found. The model parameters are listed in Table 4.4. Even though the fluid was at rest, the Reynolds number was high ($Re = 140$) as the terminal velocity of a falling particle is much higher than the fluid velocity.

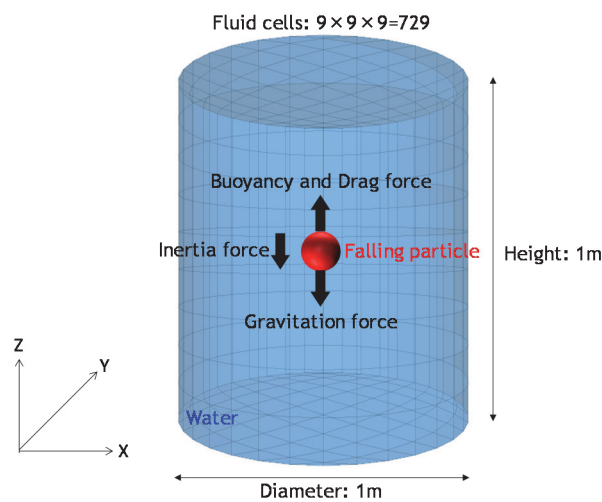


Figure 4.17 Falling particle in a static fluid

Table 4.1 Physical and geometric parameters for the column filled with water (Suzuki et al., 2007)

Parameters	Value	Unit
Solid (particle)		
Number	1	-
Diameter, d	1.00×10^{-3}	m
Density, ρ_s	2.65×10^3	kg/m ³
Fluid (water at 20°C, 1 atm)		
Density, ρ_w	1.0×10^3	kg/m ³
Viscosity, μ_f	1.004×10^{-3}	Pa·s
Column configuration		
Height	1	m
Diameter	1	m
Calculation		
Gravity, g	9.80665	m/s ²
Time step for particle, Δt_p	1.0×10^{-5}	s
Time step for fluid, Δt_f	1.0	s
Time step for data exchange, Δt_e	1.0×10^{-2}	s
Number of fluid cells	9×9×9	cells

To develop the analytical solution for this problem, forces that are acting on a falling particle are divided into four forces: inertia, gravitation, buoyancy and drag force as shown in Figure 4.17. Referring to the PFC manual (Itasca Consulting Group, 2007), the equation of motion of a falling particle in a fluid using Newton's second law can be described by:

$$\frac{4}{3}\pi r^3 \rho_p \frac{dv_z}{dt} = \frac{4}{3}\pi r^3 (\rho_p - \rho_f)g - \frac{1}{2}\pi r^2 \rho_f C_D v_z^2 \quad 4.13$$

where r is particle radius; v_z is vertical velocity of falling particle; ρ_p is particle density; and g is acceleration due to gravity. The gradient ($\frac{dv_z}{dt}$) approaches zero as the falling particle reaches a terminal velocity; at this point, Equation 4.13 becomes:

$$\frac{1}{2}\pi r^2 \rho_f C_D v_z^2 = \frac{4}{3}\pi r^3 (\rho_p - \rho_f)g \quad 4.14$$

In this verification, the Di Felice equation (Equation 4.8) was used to calculate drag forces

under turbulent flow separation with a full range of Reynolds number. For a falling spherical particle with a radius of 0.5 mm and a particle density of 2,650 kg/m³ under gravity (9.8 m/s²) in water with a fluid density of 1,000 kg/m³ and a fluid viscosity of 1.004E-3 Pa·s, Equation 4.8 gives C_D of 1.07, and then a velocity of 0.142 m/s is calculated as shown in Figure 4.18.

In the coupled PFC3D-CCFD model created here, a cylinder with a height of 1m and a diameter of 1 m was considered. This was divided into 729 hexahedral elements using the PFC3D-CCFD program. The boundary conditions along the circumference and bottom of the cylinder were specified to be free slip boundary conditions. A constant pressure condition of $P = 0$ was applied to the top boundary. A particle with the diameter of 1 mm was initially placed 0.2 m below the top surface of the cylinder. The physical parameters were the same as those applied to Equation 4.14 above. The particle accelerated under gravity to achieve a terminal velocity when the drag and gravitation forces equilibrated. The time step for particles was set to be smaller than the critical time step for solution stability, which is approximately calculated at 1E-6 numerical seconds from Equation 3.1, and the time step for water and data exchange was specified to be 1E-3 numerical seconds. The model was run for 0.2 numerical seconds. The results for the simulated model solution using the PFC3D-CCFD program are shown in Figure 4.18. The model correctly captures the correct terminal velocity of the particle, which is 0.142 m/s after 0.1 numerical seconds of coupled calculation, i.e. the analytical result is the same as the simulated result. In Figure 4.19, both analytical and simulated drag force are shown. Here, the analytical drag force is 8.46E-6 N after 0.1 numerical seconds, whereas the simulated one is 8.47E-6 N, so there is a slight difference between these results.

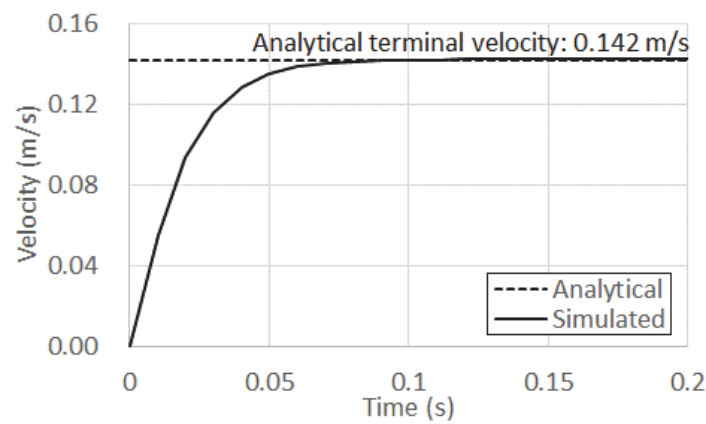


Figure 4.18 Terminal velocity

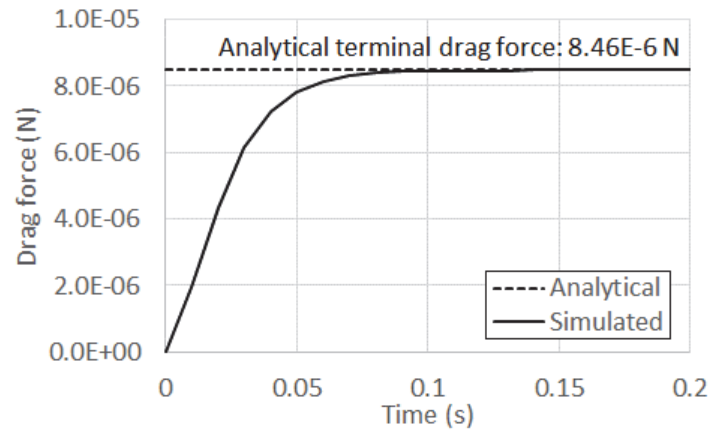


Figure 4.19 Terminal drag force

In addition to this result, the effect of time increments and mesh sizes on the accuracy of simulation were considered as shown in Table 4.2 and Table 4.3. The time increments have only a slight effect on the accuracy (the seventh decimal place) as shown in Figure 4.20. Mesh sizes affect the accuracy slightly too (the sixth decimal place). From these results for the time increments and mesh sizes considered, the effect of mesh sizes seem to be a little bit bigger than that of time increments. As shown in Figure 4.21, the error increases with the number of fluid cells; however, the error is still less than 0.1%. In practical terms, there is almost no effect on the time increments and mesh sizes as the error is very low.

Table 4.2 Effects of different time steps

Time step (seconds)			Elements	Particle diameter/ Cell height	Terminal velocity (m/s)	Error (%)
DEM	Data exchange	CFD				
1E-5	1E-1	1E-1	729 (9×9×9)	0.009	0.1421321582241145	0.0931
	1E-2	1E-2			0.1421321248804937	0.0930
	1E-3	1E-3			0.1421322591198505	0.0931
	1E-4	1E-4			0.1421322680288070	0.0931
	1E-5	1E-5			0.1421325001493202	0.0933
1E-6	1E-1	1E-1	729 (9×9×9)	0.009	0.1421321570081745	0.0931
	1E-2	1E-2			0.1421330680682871	0.0937
	1E-3	1E-3			0.1421322478719672	0.0931
	1E-4	1E-4			0.1421322681736751	0.0931
	1E-5	1E-5			0.1421323364767308	0.0932
	1E-6	1E-6			0.1421326068873840	0.0934
1E-7	1E-1	1E-1	729 (9×9×9)	0.009	0.1421321569164265	0.0931
	1E-2	1E-2			0.1421321205096986	0.0930
	1E-3	1E-3			0.1421322479421864	0.0931
	1E-4	1E-4			0.1421322599351387	0.0931
	1E-5	1E-5			0.1421322687389439	0.0931
	1E-6	1E-6			0.1421323543666028	0.0932
	1E-7	1E-7			0.1421323750725342	0.0932

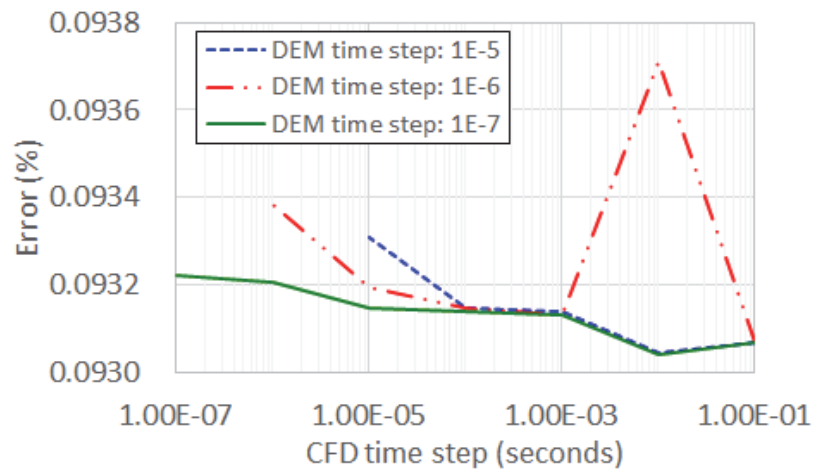


Figure 4.20 Error with different DEM time steps

Table 4.3 Effects of different mesh sizes

DEM	Time step (seconds)		Elements	Particle diameter/ Cell height	Terminal velocity (m/s)	Error (%)
1E-6	1E-1	1E-1	125 (5×5×5)	0.005	0.1421322165352991	0.0931
			729 (9×9×9)	0.009	0.1421321570081745	0.0931
			8,000 (20×20×20)	0.020	0.1421314407652748	0.0926
	1E-2	1E-2	125 (5×5×5)	0.005	0.1421320639637537	0.0930
			729 (9×9×9)	0.009	0.1421330680682871	0.0937
			8,000 (20×20×20)	0.020	0.1421351958930192	0.0952
	1E-3	1E-3	125 (5×5×5)	0.005	0.1421322691709202	0.0932
			729 (9×9×9)	0.009	0.1421322478719672	0.0931
			8,000 (20×20×20)	0.020	0.1421356898643369	0.0956
	1E-4	1E-4	125 (5×5×5)	0.005	0.1421323001275787	0.0932
			729 (9×9×9)	0.009	0.1421322681736751	0.0932
			8,000 (20×20×20)	0.020	0.1421357562282808	0.0957
	1E-5	1E-5	125 (5×5×5)	0.005	0.1421324021542803	0.0932
			729 (9×9×9)	0.009	0.1421323364767308	0.0932
			8,000 (20×20×20)	0.020	0.1421359084874935	0.0957
	1E-6	1E-6	125 (5×5×5)	0.005	0.1421325109623516	0.0933
			729 (9×9×9)	0.009	0.1421326068873840	0.0934
			8,000 (20×20×20)	0.020	0.1421334459400196	0.0940

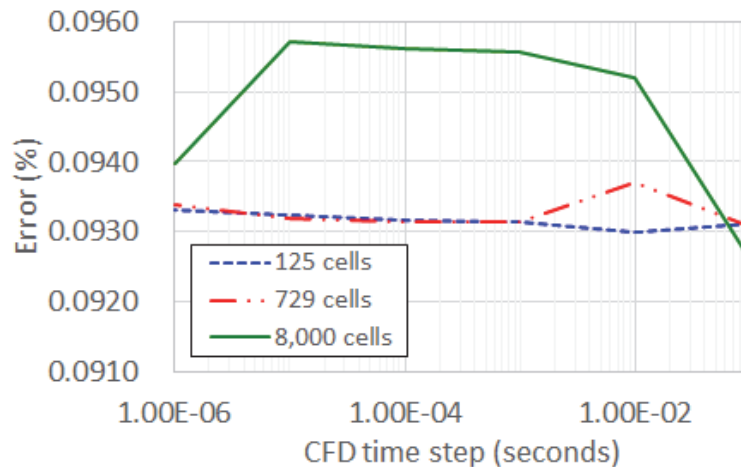


Figure 4.21 Error with different number of fluid cells

4.5.2. Multiple particle system

To validate the PFC3D-CCFD program for a case with multiple particles, a one dimensional

system, which was previously investigated by Suzuki et al. (2007), was considered. In this validation, 100 spherical particles were vertically placed in a square column, which filled with water. This square column configuration is shown in Figure 4.13. The size of a fluid cell differs from the fluid cell size used by Suzuki et al. (2007). According to Itasca Consulting Group (2007), the length of each fluid cell should be at least five particle diameters. Thus, five particles are in one fluid cell as shown in Figure 4.13. In addition, there are two cavity (i.e. empty) fluid cells at both ends of the column to get a stable water flow and hydraulic gradient at each end. In this validation, the upward displacement of the particles, the excess pore water pressure distribution in the square column and critical hydraulic gradient were considered. The model parameters are listed in Table 4.4. These parameters are exactly the same as ones used in the work of Suzuki et al. (2007) except the height of a fluid cell, which is five times as large as that used in the work of Suzuki et al. (2007). The numerical model here differs from the model considered by Suzuki et al. (2007); they used the Ergun drag expression rather than the Di Felice expression and so a modified analytical validation had to be derived.

Table 4.4 Physical and geometric parameters for the column filled with water (Suzuki et al., 2007)

Parameters	Value	Unit
Solid (particle)		
Number	100	-
Diameter, d	1.0×10^{-3}	m
Density, ρ_s	2.65×10^3	kg/m ³
Spring constant, k_n	1.0×10^2	N/m
Fluid (water at 20°C, 1 atm)		
Density, ρ_w	1.00×10^3	kg/m ³
Viscosity, μ_f	1.004×10^{-3}	Pa·s
Water flow	0.005, 0.01, 0.018	m/s
Column configuration		
Height	0.1	m
Width	1.0×10^{-3}	m
Length	1.0×10^{-3}	m
Calculation		
Gravity, g	9.80665	m/s ²
Time step for particle, Δt_p	1.0×10^{-5}	s
Time step for fluid, Δt_f	1.0×10^{-3}	s
Time step for data exchange, Δt_e	1.0×10^{-3}	s
Fluid cell size	5.0×10^{-3}	m

In the analytical solution, the problem of one-dimensional upward seepage flow was simulated in three stages: a consolidation stage, a swelling stage and a water flow stage. During the consolidation process, particles settle down under gravity and buoyancy forces. The settlement of the top particle can be expressed by:

$$\delta = \frac{N_p(N_p + 1)}{2} \frac{f_i}{k_n} \quad 4.15$$

$$f_i = \frac{4\pi r^3}{3} \rho_{sat} \quad 4.16$$

where δ is the amount of settlement of the top particle; f_i is the force per particle; k_n is spring constant (in the contact normal direction); and ρ_{sat} is submerged density ($\rho_{sat} = \rho_p - \rho_w$). After the first stage of consolidation, water flow is applied from the bottom boundary. The water flow velocities considered are 0.005, 0.010 and 0.018 m/s. According to the consolidation theory that was proposed by Terzaghi (1943), the following assumptions are made: (a) the soil is isotropic and homogeneous, and the voids are completely saturated, (b) the particles and fluid are incompressible, (c) the compression and water flow are one dimensional, (d) hydraulic gradients are based on Darcy's law, (e) the relationship between the void ratio and effective stress is linear in an e - $\log P$ diagram, and (f) the coefficient of permeability and volume compressibility do not change throughout the process. Consolidation in one dimension can then be described as:

$$\frac{\partial u_e}{\partial t} = C_v \frac{\partial^2 u_e}{\partial z^2} \quad 4.17$$

where u_e is the excess pore water pressure; and C_v is the coefficient of consolidation, which is given by:

$$C_v = \frac{k}{m_v \rho_w g} \quad 4.18$$

where m_v is coefficient of volume compressibility; ρ_w is fluid density as before; and g is acceleration due to gravity as before. The movement of the top surface can be given by integrating the strain:

$$S_t = - \int_0^H \epsilon dz = - \int_0^H m_v \Delta P' dz = - \int_0^H m_v u_e dz \quad 4.19$$

where S_t is the movement of the top surface; H is thickness of soil layer; ϵ is the strain; and $\Delta p'$ is the increment in mean effective stress. According to the work of Suzuki et al. (2007), adopting the analytical solution for thermal conduction problems, u_e can be calculated as:

$$u_e = H \rho_w g \frac{v_f}{k} \left(\frac{z}{H} - \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2} \sin \left(\frac{(2n+1)\pi z}{2H} \right) \exp(-T_v(2n+1)^2 \pi^2 / 4) \right) \quad 4.20$$

where v_f is fluid velocity as before; and T_v is dimensionless time factor, which in the case of single drainage is given by:

$$T_v = \frac{C_v t}{H^2} \quad 4.21$$

By substituting Equation 4.20 into Equation 4.19, upward displacement (S_t) by swelling can be obtained as:

$$S_t = \frac{v_f H^2}{C_v} \frac{1}{2} \left(1 - \frac{32}{\pi^3} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^3} \exp(-T_v(2n+1)^2 \pi^2 / 4) \right) \quad 4.22$$

In the validation described by Suzuki et al. (2007), the expression for the dissipation of excess pore water pressure is derived using the Ergun equation for the pressure drop through a granular material (Equation 4.7):

$$\frac{\Delta P}{H} = \frac{1-n}{dn^3} \left(150 \frac{(1-n)\mu_f v_f}{d} + 1.75 \rho_w v_f^2 \right) \quad 4.23$$

where ΔP is fluid pressure difference; d is particle diameter as before; and μ_f is fluid viscosity as before. When the Di Felice equation (Equation 4.8) is used instead of the Ergun equation, the dissipation of excess pore water pressure is given by:

$$\frac{\Delta P}{H} = \frac{3C_{D0}(1-n)\rho_w v_f^2}{4nd} n \left(3.7 - 0.65 \exp \left(\frac{-(1.5 - \log(Re))^2}{2} \right) \right) \quad 4.24$$

The hydraulic gradient (i) is given by:

$$i = \frac{\Delta h}{H} = \frac{\Delta P}{\rho_w g H} \quad 4.25$$

where Δh is head difference. From Equations 4.23 to 4.25, permeability is shown in two different forms of equations as:

$$\text{Ergun} \quad k = \frac{v_f}{i} = \frac{v_f \rho_w g}{\frac{1-n}{dn^3} \left(150 \frac{(1-n)\mu_f v_f}{d} + 1.75 \rho_w v_f^2 \right)} \quad 4.26$$

$$\text{Di Felice} \quad k = \frac{4nd\rho_w g v_f}{3C_{D0}(1-n)\rho_w v_f^2 n \left(3.7 - 0.65 \exp \left(\frac{-(1.5 - \log(Re))^2}{2} \right) \right)} \quad 4.27$$

these equations are substituted into Equation 4.18 to obtain C_v .

As mentioned above, Terzaghi's theory is adopted when upward displacement by swelling is calculated. The theory is an analytical solution for a porous continuum, based on the heat equation. Accordingly, it is not an analytical solution for DEM, and an exact result is not expected here. In the simulation, gravity was firstly applied to all balls in an uncoupled DEM simulation stage. Once the settlement of all particles became stable when tolerance is smaller than 1E-6, water was applied to the square column and the particles were again allowed to stabilise. Here, the settlement under gravitational force was obtained using Equations 4.15 and 4.16, i.e. the theoretical value calculated from these equations is 0.0004279 m at 10 seconds as shown in Figure 4.22. This result is in good agreement with simulated result in the PFC3D-CCFD program. As mentioned in Section 4.4.5 and shown in Figure 4.22, all balls are fixed at 12 seconds just before water flow is applied from the bottom. Then, all balls are released at 15 seconds. The results for the swelling stage after 12 seconds are considered below.

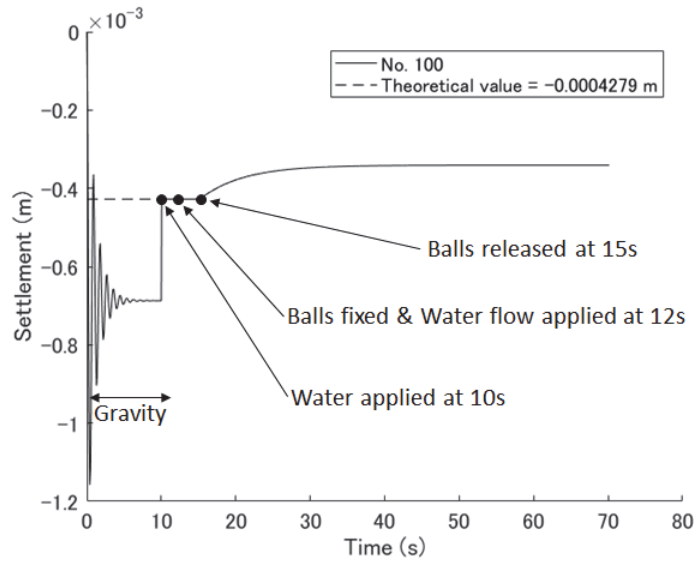


Figure 4.22 Settlement of top ball with time

In the swelling stage, the upward displacement by using Equation 4.22 was obtained as shown in Figure 4.23. The simulated upward displacement (0.0000870 m) after applying water flow of 0.005 m/s agrees well with the analytical upward displacement (0.0000877 m) calculated by the Di Felice equation. In this validation model, the porosity is 0.4764 (void ratio is 0.9099). Judging from Figure 4.4, the drag force calculated by the Di Felice equation is lower than that calculated by the Ergun equation by approximately 15%. This fact agrees with the data in Figure 4.23; the Di Felice drag gives less displacement.

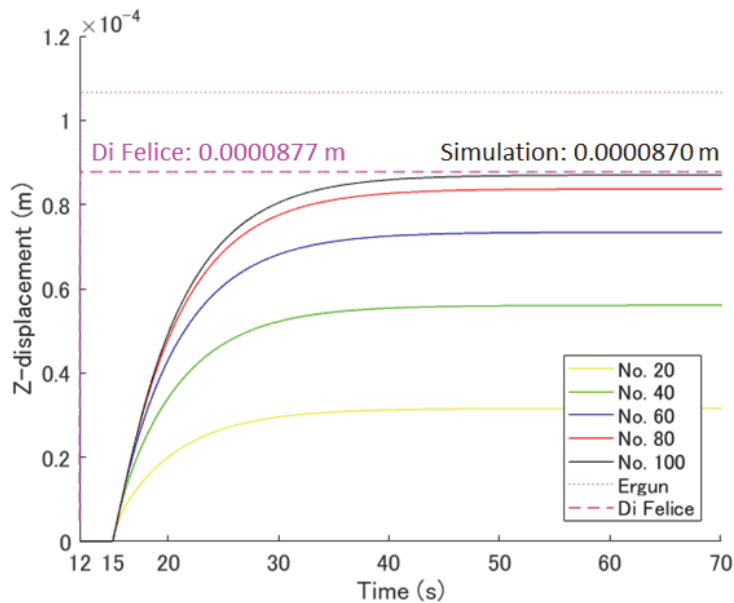


Figure 4.23 Displacement after applying water flow of 0.005 m/s

The comparison of upward displacement of top ball (No. 100) under different water flow velocities between analytical and simulated values is shown in Table 4.5. All simulated values are in good agreement with the analytical values.

Table 4.5 Comparison of upward displacement between analytical and simulated values

Water flow velocity (m/s)	Upward displacement of top ball (No.100) (m)		Error (%)
	Simulated	Analytical	
0.005	0.0000870	0.0000877	0.8
0.010	0.0001936	0.0001952	0.8
0.018	0.0004080	0.0004084	0.1

The excess pore water pressure can be calculated by using Equations 4.20, 4.26 and 4.27. When the water flow of 0.005 m/s is applied, the excess pore water pressure distribution obtained from the simulation and calculated by both the Di Felice equation and the Ergun equation is described in Figure 4.24. Although the simulated values tend to be lower than those theoretically calculated from the Di Felice equation, both simulated and analytical values are close; on the other hand, the excess pore water pressure calculated by the Ergun equation is larger than that calculated by the Di Felice equation. The difference between these results is 17%, which is in good agreement with the difference in Figure 4.23. However, an exact match between simulated and analytical results is not expected since Terzaghi's theory is not designed for DEM.

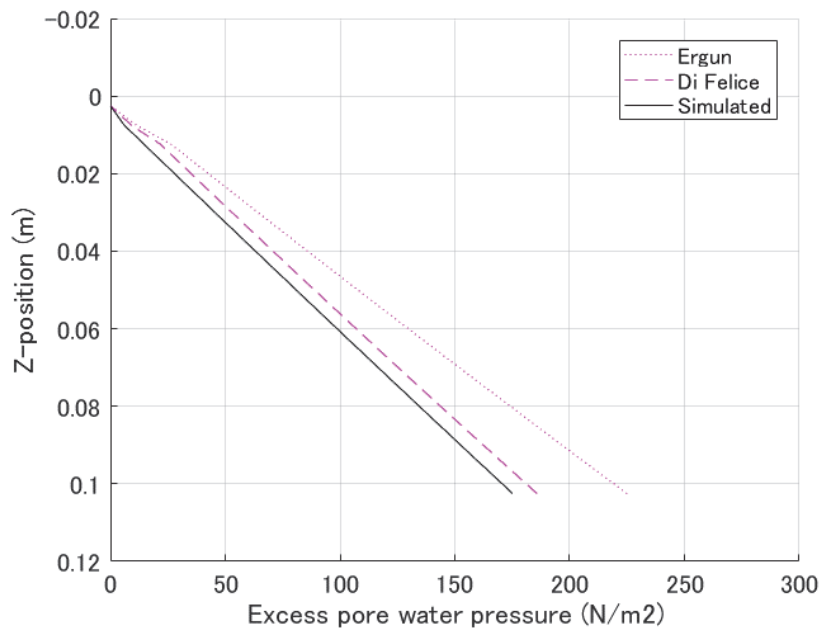


Figure 4.24 Excess pore water pressure distribution at 70 seconds

The comparison of excess pore water pressure between simulated and analytical values is shown in Table 4.6 when the velocity of water flow is varied. Although the simulated values tend to be smaller than the analytical values, the difference between these values is small. Therefore, it is clearly found that the coupled PFC3D-CCFD software is useful to accurately simulate the behaviour of soil particles and water.

Table 4.6 Comparison of excess pore water pressure at bottom between analytical and simulated values

Water flow velocity (m/s)	Excess pore water pressure at bottom (N/m ²)		
	Simulated	Analytical (Di Felice)	Error (%)
0.005	175	186	5.7
0.010	388	407	4.7
0.018	809	831	2.6

Chapter 5. MAIN SIMULATIONS

5.1. Introduction

Building on the concepts presented in Chapter 2 to Chapter 4, in this chapter coupled DEM-CFD models are developed and applied to examine the initiation of internal instability under a specified confining pressure and hydraulic gradient. Section 5.2 introduces the simulation configuration and discusses the parameters that were selected for monitoring. Section 5.3 presents the results of the simulations using four samples that are expected to have different susceptibilities to internal instability. Section 5.4 synthesises the results and draws conclusions.

5.2. Virtual permeameter configuration

5.2.1. Simulation configuration

Before the main virtual permeameter tests were started, a prototype sample was used to develop the simulation procedure. The prototype sample was created using the compression method described in Section 3.3.1, i.e. it was isotropically compressed and gravity was applied in five stages. As illustrated in Figure 5.1, the prototype sample comprised 1,000 particles with a Cu of 1.2. As $\mu = 0.3$, the sample was loose. The prototype sample parameters used here are listed in Table 5.1. The simulation process is given in Figure 5.2. Referring to Figure 5.3 (a), it was relatively homogeneous. As illustrated in Figure 5.3, fluid cells were created (Figure 5.3 (b)) after sample compression. The fluid cells at each end in the vertical direction were extended by one fluid cell to avoid an abrupt change in fluid flow (Figure 5.3 (c)). Once the particles and the fluid cells were coupled, i.e. once the PFC3D and CCFD software programs were linked, initial and boundary conditions were applied to the whole system. The boundary condition for the lateral fluid cells was set to be a free slip condition as was illustrated in Figure 4.6. In the vertical direction, a fluid pressure of 0 N/m² was applied on a top fluid cell, and a specified fluid pressure was applied to a bottom fluid cell. For the prototype simulation, the lower boundary applied pressure was always 10 Pa. A user defined function for applying pressure boundary conditions was developed by Jason Furtney at Itasca in January 2016 so that the hydraulic gradient could easily be changed during the simulation process. The user defined function needs to be compiled with Visual Basic Studio 2015 (the product of Microsoft) before it is used as mentioned in Section 4.4.4 and is given in Appendix A.

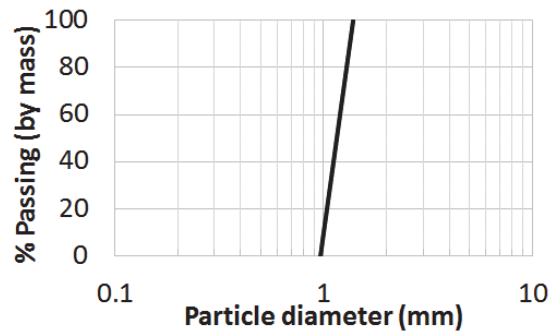


Figure 5.1 PSD for prototype sample with $Cu = 1.2$

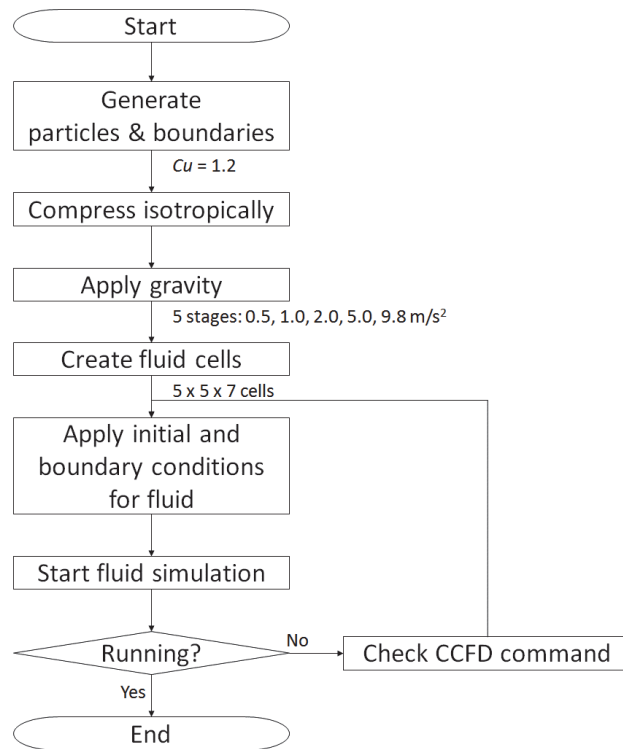


Figure 5.2 Flowchart of prototype simulation process

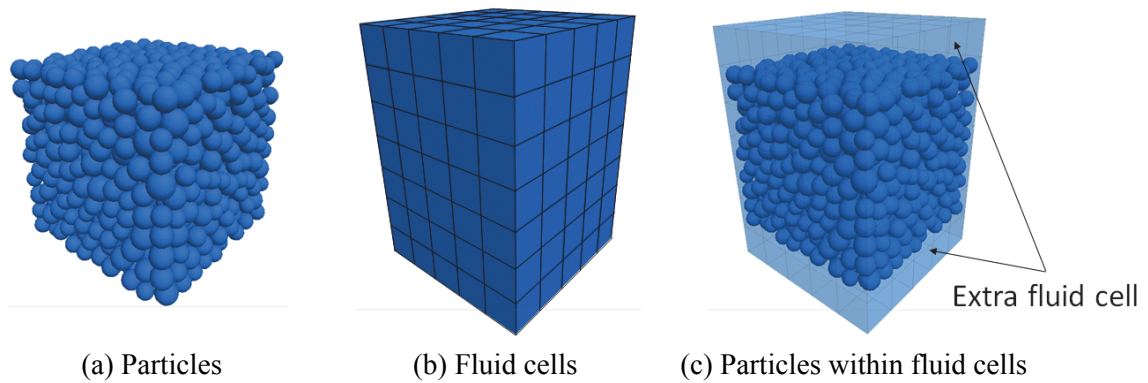


Figure 5.3 Schematic figures of 1,000 particles and fluid cells

Table 5.1 Physical and geometric parameters for prototype samples

Parameter values	Unit	1,000 particles
Soil particle		
Diameter, d	m	$9.64 \times 10^{-4} - 1.39 \times 10^{-3}$
Density, ρ_s	kg/m ³	2.67×10^3
Poisson's ratio, ν	-	0.3
Shear modulus, G	GPa	27.0
Coefficient of friction, μ		
between particles	-	0.3
between particles and walls	-	0.0
Local damping		0.05
Contact model	-	Non-linear Hertz-Mindlin
Boundary condition	-	
top boundary	-	Fluid pressure, $P = 0$ Pa
lateral boundary	-	Free slip
bottom boundary	-	Fluid pressure $P = 10$ Pa
Fluid (water at 20 °C, 1 atm)		
Density, ρ_w	kg/m ³	1.00×10^3
Viscosity, μ_f	Pa · s	1.004×10^{-3}
Column configuration		
Height	m	1.6×10^{-2}
Width	m	1.1×10^{-2}
Depth	m	1.1×10^{-2}
Numerical calculation		
Gravity, g	m/s ²	9.80665
Time step for particle, Δt_p	s	2.0×10^{-8}
Time step for fluid, Δt_f	s	1.0×10^{-3}
Time step for data exchange, Δt_e	s	1.0×10^{-3}
Fluid cell size	m	2.2×10^{-3}

Once it was confirmed that the prototype sample simulations could run effectively (i.e. continuity or conservation of fluid mass was achieved), the main virtual permeameter tests were considered. As mentioned in Chapter 3, four samples, whose PSDs are given in Figure 3.1, were used: a loose sample with 25% fines content, a dense sample with 25% fines content, a loose sample with 35% fines content, and a dense sample with 35% fines content. As illustrated in Figure 5.4 (a), particles were randomly placed in non-touching positions and then the samples were compressed to 50 kPa under isotropic compression as shown in Figure 5.4 (b). Then, fluid cells were created and the boundary conditions for the fluid were specified as given in Figure 5.4 (c). As mentioned above, both ends of fluid mesh were extended vertically by one fluid cell as shown in Figure 5.3 (c). After the fluid flow was deemed to have converged, all the relevant information was recorded. When a small number of particles are used in simulations, the particle positions had to be fixed for a while to avoid abrupt changes in water velocity linked to numerical oscillation as mentioned in Section 4.4.4. However, particles do not need to be fixed for the large number of particles in these simulations since there is no numerical oscillation after applying a specified hydraulic gradient. It is not clear why there was this difference in simulations as a result of difference in sample size. For these large simulations, a specified hydraulic gradient was applied and maintained constant for a controlled duration. At the beginning of each simulation, a hydrostatic water pressure condition was applied over 0.10 numerical seconds to the whole system, i.e. $i = 0$. It was confirmed that there was no change in the coordination number Z over this time period. Once this condition was achieved, the hydraulic gradient was applied by increasing the pressure at the bottom fluid cell using the user defined function mentioned above, so upward seepage flow was generated. A criterion was selected to decide when to increase hydraulic gradient. For the samples, at each simulation stage, the change in the coordination number (ΔZ) over 0.01 numerical seconds was confirmed to be smaller than 0.5% of the current coordination number (Z), i.e. $\frac{Z_t - Z_{t-0.01}}{Z_t} < 0.005$, before simulation progressed to the next stage and the hydraulic gradient was increased. The hydraulic gradients applied for the loose samples were $i = 1, 2, 10$, and those for the dense samples were $i = 1, 5, 10$. Before proceeding to a subsequent stage, a save file was created as explained in Section 4.4.4. The whole process is shown in Figure 5.5, and the parameters for the main virtual permeameter tests are listed in Table 5.2.

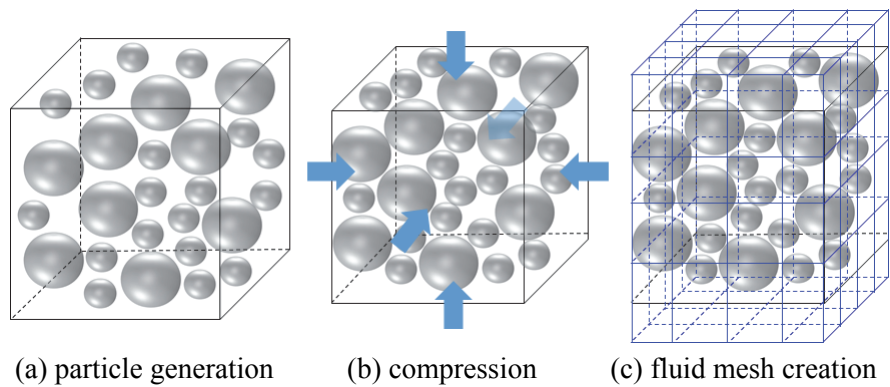


Figure 5.4 Schematic process for coupled simulation

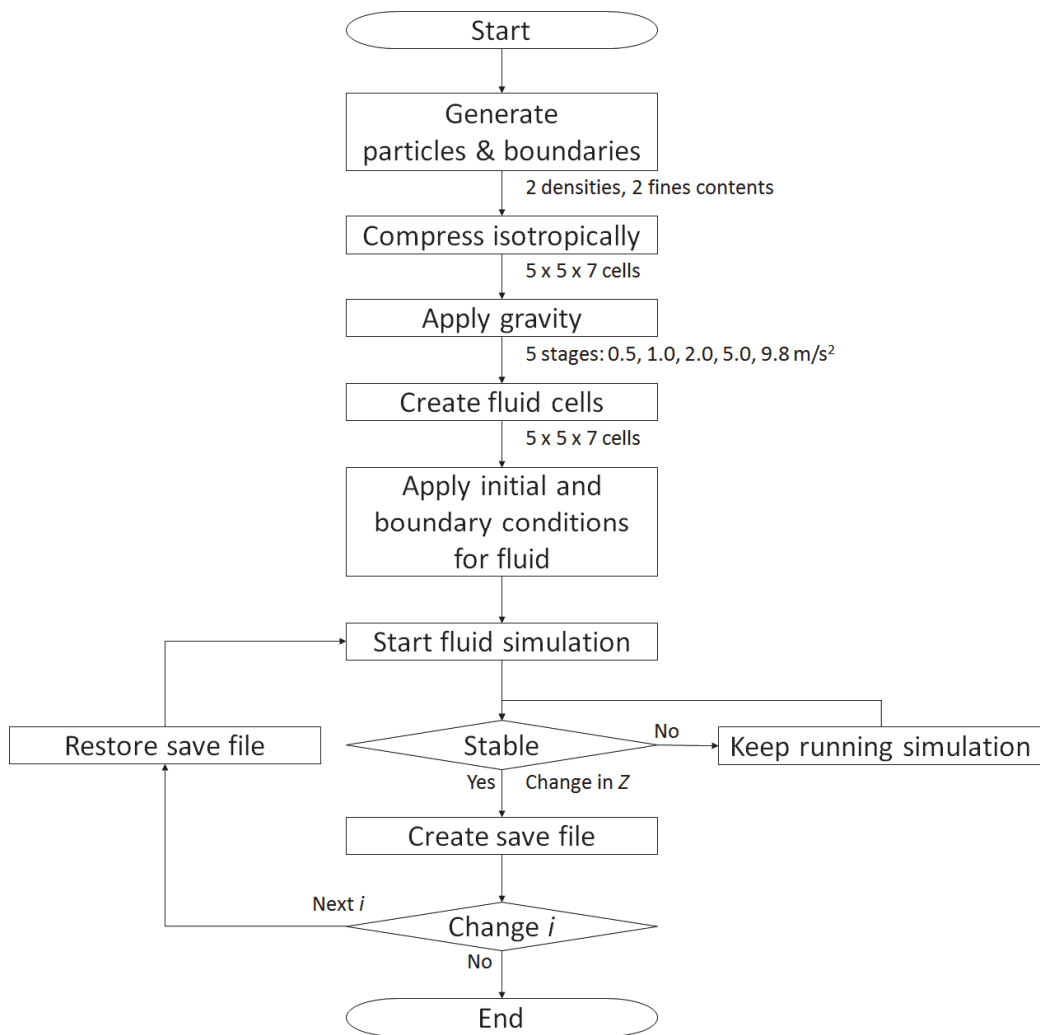


Figure 5.5 Flowchart of virtual permeameter tests

Table 5.2 Parameters for virtual permeameter tests

Parameter values	Unit	Large-loose		Large-dense	
Soil particle					
Fines content	%	25	35	25	35
Diameter, d	m	$1.2\times10^{-4}-1.0\times10^{-3}$			
Density, ρ_s	kg/m ³	2.67×10^3			
Poisson's ratio, ν	-	0.3			
Shear modulus, G	GPa	27.0			
Coefficient of friction, μ					
between particles	-	0.3			
between particles and walls	-	0.0			
Local damping		0.05			
Contact model	-	Non-linear Hertz-Mindlin			
Boundary condition	-				
top boundary	-	Fluid pressure, $P=0$ Pa			
lateral boundary	-	Free slip			
bottom boundary					
fluid pressure, P	Pa	0, 79, 159, 794	0, 84, 169, 843	0, 78, 392, 783	0, 84, 418, 835
hydraulic gradient, i	-	0, 1, 2, 10	0, 1, 2, 10	0, 1, 5, 10	0, 1, 5, 10
Fluid (water at 20 °C, 1 atm)					
Density, ρ_w	kg/m ³	1.00×10^3			
Viscosity, μ_f	Pa·s	1.004×10^{-3}			
Column configuration					
Height	m	8.1×10^{-3}	8.5×10^{-3}	8.0×10^{-3}	8.6×10^{-3}
Width	m	5.8×10^{-3}	6.1×10^{-3}	5.7×10^{-3}	6.1×10^{-3}
Depth	m	5.8×10^{-3}	6.1×10^{-3}	5.7×10^{-3}	6.1×10^{-3}
Numerical calculation					
Gravity, g	m/s ²	9.80665			
Time step					
for particle, Δt_p	s	2.0×10^{-8}			
for fluid, Δt_f	s	1.0×10^{-5}			
for data exchange, Δt_e	s	1.0×10^{-5}			
Fluid cell size	m	1.2×10^{-3}	1.2×10^{-3}	1.1×10^{-3}	1.2×10^{-3}

5.2.2. Particle-scale analyses

In order to assess whether internal instability had occurred, some specific data were selected to monitor how particle migration was proceeding. Displacement was the main parameter used to identify and quantify particle migration. The particle displacement is defined as:

$$d_{particle} = \sqrt{(\Delta x^2 + \Delta y^2 + \Delta z^2)} \quad 5.1$$

where $d_{particle}$ is the displacement between the initial and final positions; Δx is the difference between the initial and final positions in the x direction; Δy is the difference between the initial and final positions in the y direction; and Δz is the difference between the initial and final positions in the z direction. The coordination number (Z) (Equation 3.2) was also considered. The magnitude of the coordination number shows the contact density within a sample, so dense samples have a large coordination number. The connectivity ($C_{particle}$) is defined as the number of contacts per each particle as shown in Figure 5.6. Particle migration due to seepage flow is expected to be linked to connectivity (Fell et al., 2005). From the structural and geometric view, particles with $C_{particle} < 4$ are regarded to be statically unstable, i.e. particles with lower connectivity are likely to be more erodible, whereas particles with $C_{particle} \geq 4$ are regarded to be statically redundant. These particles with $C_{particle} \geq 4$ surrounded by other particles cannot move around because of the lack of space (Zhang & Makse, 2005). Note that the average or mean connectivity ($C_{particle}$) is equal to the coordination number (Z).

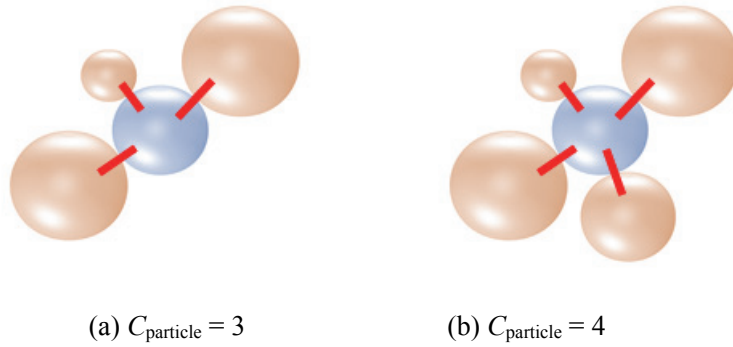


Figure 5.6 Schematic figures of connectivity

5.3. Overall system response

5.3.1. Analysis of permeability

The permeability of the four samples was calculated by Equation 2.1 and the simulation data. There was some variation in permeability between application of the fluid flow and the point where the stable state was attained as illustrated in Figure 5.7. The variation was most

significant for the Gap25_Loose sample. For this sample, the permeability dramatically decreases during the simulation from 6.1×10^{-4} m/s to 2.3×10^{-4} m/s (Figure 5.7 (a)). At the end of the simulation, the permeability of this sample is approximately twice that of the other samples. This is reflected in the large fluid flow observed soon after applying a hydraulic gradient (i) of one as given in Figure 5.8 (a). According to Darcy's law, $v = ki$, so any changes in permeability are accompanied by changes in velocity, resulting in the change of fluid flow. The other samples also exhibited a decrease in permeability during the simulations; however, this decrease was smaller. As would be expected the permeability of Gap25_Dense was less than the permeability of Gap25_Loose and similarly the permeability of Gap35_Dense was less than that of Gap35_Loose.

It is essential to compare the simulated results with empirical values and experimental data so that the results obtained from simulations are validated. As suggested in Equation 4.27, permeability can be empirically calculated using the Di Felice equation. In addition to the Di Felice equation (Equation 4.27), the Ergun equation (Equation 4.26), the Hazen equation (Equation 2.6) and the Chapius equations (Equation 2.7) are also used to determine expected values as in the work of Jeyisanker & Gunaratne (2009) that is mentioned in Section 2.3.1. Using the porosity values given in Table 3.2, the permeability values from the simulations at the stable state and expected values calculated from Equation 4.27 are listed in Table 5.3 and Figure 5.9. The slopes of plots of discharge velocity ($v_{\text{discharge}}$) versus hydraulic gradient (i) are also included. These data are discussed further below. The experimental data of Slangen (2015) are also given.

Referring to Figure 5.9, although there is some discrepancy between the values obtained from the simulations and the empirical values, it is found that all results agree with in one order of magnitude. The permeability obtained from the Hazen equation is in quite good agreement with the simulated permeability, while the permeability values obtained from the Chapius equation are the lowest amongst all the permeability values. Note that the Hazen and Chapius equations use D_{10} . The values from the Di Felice and the Ergun equations do not give as good agreement with the simulated permeability values. They depend on the median diameter (D_{50}) rather than D_{10} . As mentioned in Section 3.4.1, D_{50} for gap-graded soil is assumed to be 0.5 mm. It is not clear whether there should be a simple link between D_{50} and permeability for a gap-graded soil. However, the drag force in the simulations is calculated from the Di Felice expression and so a better match was expected. Perhaps, the difference is due to sample inhomogeneity effects.

Slangen (2015) carried out experiments with gap-graded samples of spherical glass beads under various hydraulic gradient as mentioned in Section 2.2.3. The sample referred to as “4.8GB35” in his study is almost the same as the Gap35_Loose sample considered here. The 4.8GB35 sample has a porosity between 0.265 and 0.270, and the Gap35_Loose has the porosity of 0.278. According to the work of Slangen (2015), the permeability of the 4.8GB35 sample had 1.5×10^{-4} m/s. This result is almost the same as the simulated permeability of Gap35_Loose as given in Table 5.3. Accordingly, the simulated permeability values are regarded as being reasonable in comparison with the empirical permeability values and the experimental permeability values.

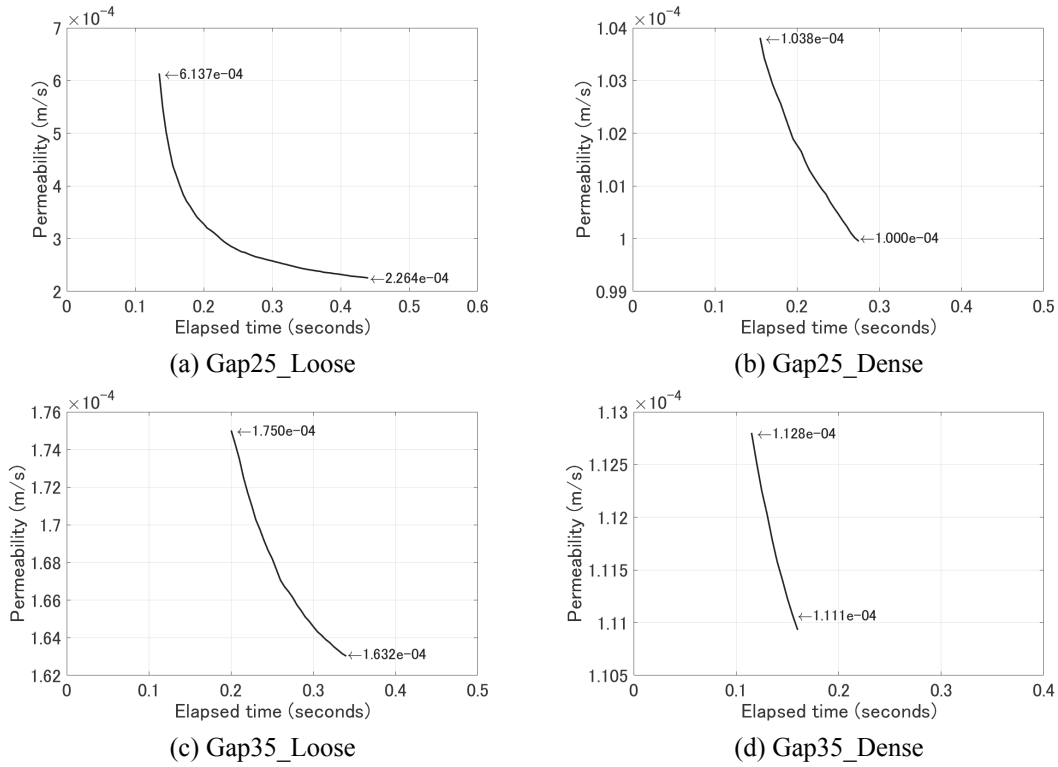


Figure 5.7 Simulated permeability under $i = 1$

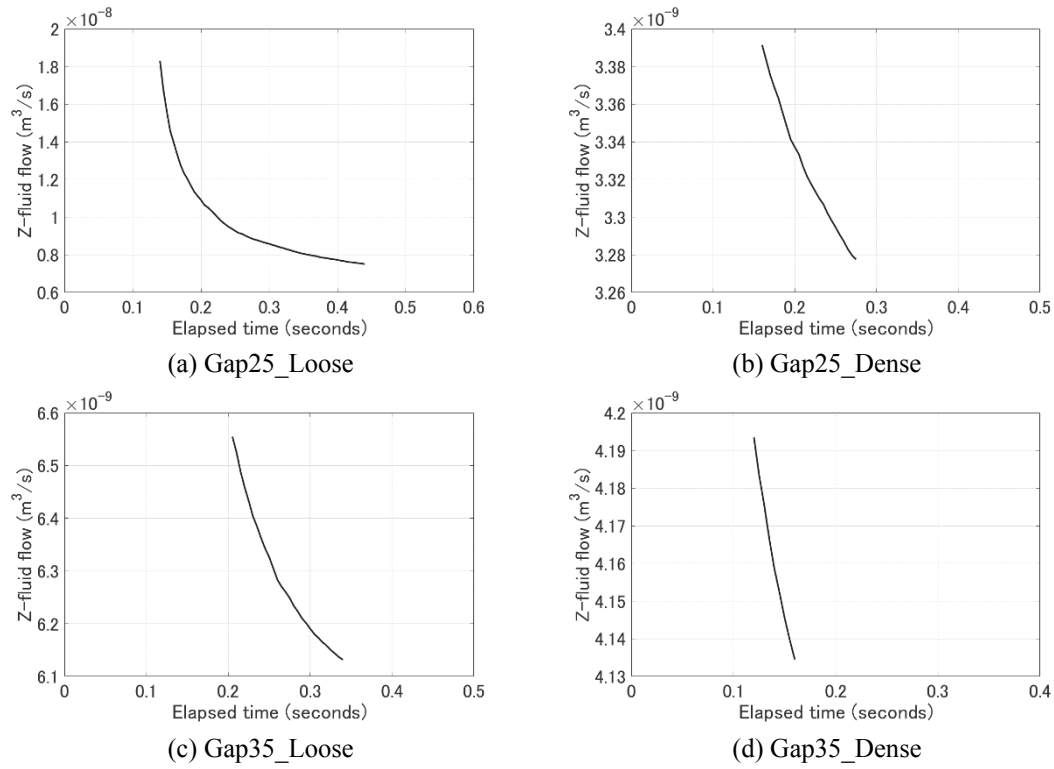


Figure 5.8 Fluid flow accompanied with permeability under $i = 1$

Table 5.3 Simulated, empirical and experimental permeability values (Note that $D_{50} = 0.5\text{mm}$)

Sample	Permeability (m/s)						Slope of $v_{\text{discharge}}$ versus i
	Simulated	Di Felice	Ergun	Hazen	Chapius	Experimental Slangen (2015)	
Gap25_Loose	2.3×10^{-4}	3.8×10^{-4}	5.8×10^{-4}	1.4×10^{-4}	6.6×10^{-5}	-	1.9×10^{-4}
Gap25_Dense	1.0×10^{-4}	2.1×10^{-4}	3.7×10^{-4}	1.4×10^{-4}	4.6×10^{-5}	-	9.6×10^{-5}
Gap35_Loose	1.6×10^{-4}	4.6×10^{-4}	6.7×10^{-4}	1.7×10^{-4}	8.3×10^{-5}	1.5×10^{-4}	1.6×10^{-4}
Gap35_Dense	1.1×10^{-4}	3.1×10^{-4}	5.0×10^{-4}	1.7×10^{-4}	6.6×10^{-5}	-	1.1×10^{-4}

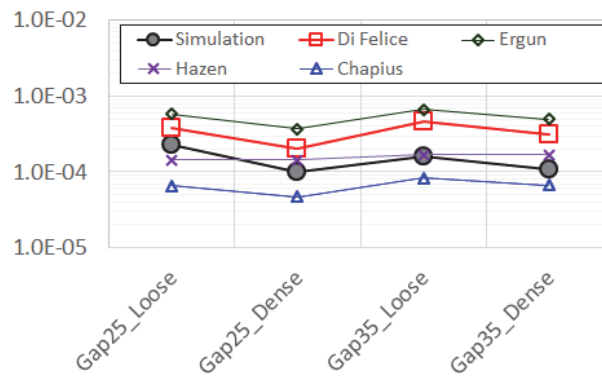


Figure 5.9 Simulated and expected permeability values

After a hydraulic gradient of $i = 1$ was applied, and the samples were deemed stable, the hydraulic gradient was further increased to a larger i . For the loose samples, i was changed to 2, and then 10, whereas for the dense samples i was increased to 5 and then 10 as well. In all samples, the permeability slightly increased soon after applying $i = 1$ and then gradually converged as shown in Figure 5.10. Hydro-mechanical properties such as the permeability and the Reynolds number (Equation 4.8) are also listed in Table 5.4. Although the permeability of each sample was not supposed to vary, the Reynolds number increased in proportion with i . Following Mitchell & Soga (2005), fluid flow under up to $Re = 10$ can be considered as having laminar flow. From the values in Table 5.4, it is obviously shown that all situations with various hydraulic gradients have laminar fluid flow.

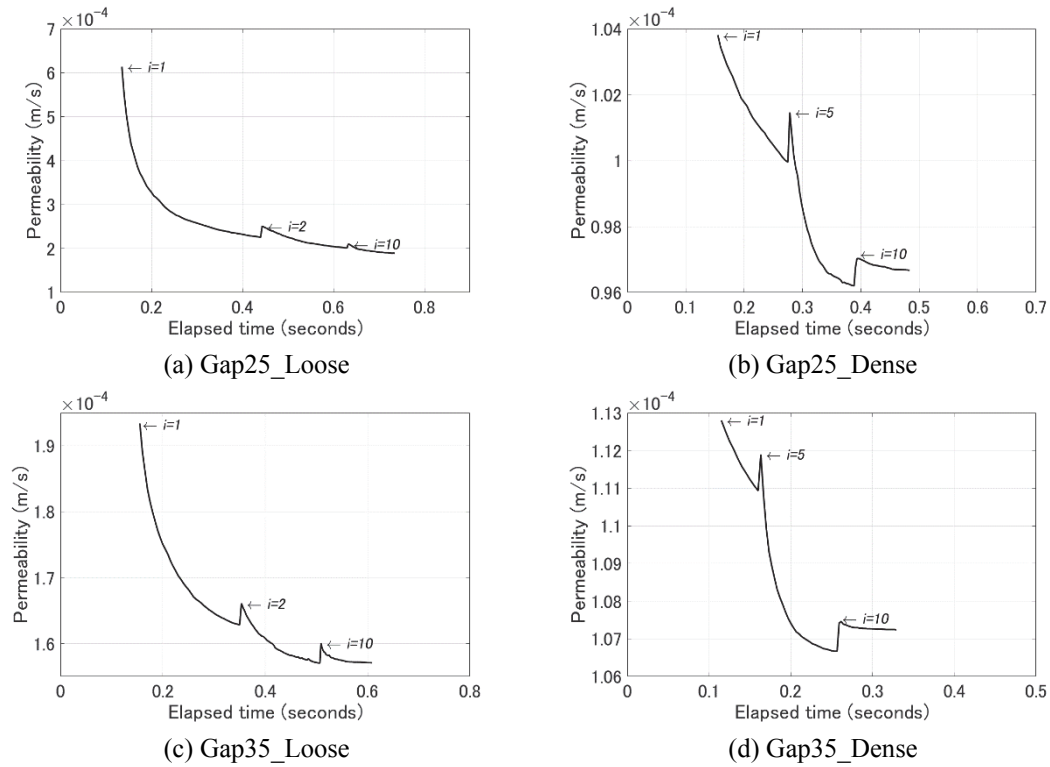
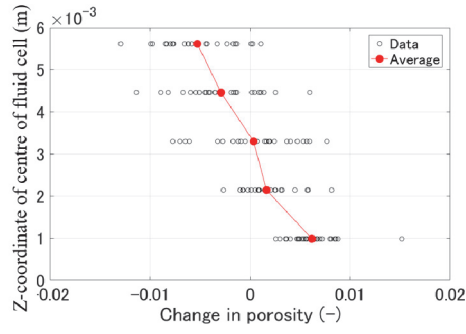


Figure 5.10 Change of simulated permeability under all i

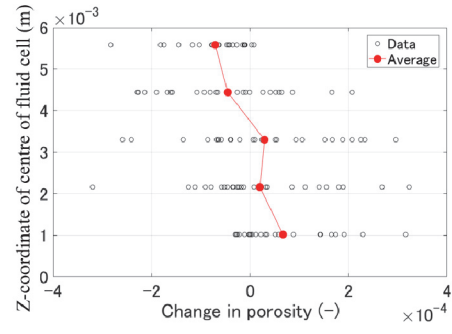
Table 5.4 Hydro-mechanical properties obtained from simulations under $i \geq 1$

Property		Gap25_Loose	Gap25_Dense	Gap35_Loose	Gap35_Dense
α, p'		0.11	0.43	0.64	1.18
Permeability (m/s)	$i = 1$	2.4×10^{-4}	1.0×10^{-4}	1.6×10^{-4}	1.1×10^{-4}
	$i = 2$	2.0×10^{-4}	-	1.6×10^{-4}	-
	$i = 5$	-	9.6×10^{-5}	-	1.1×10^{-4}
	$i = 10$	1.9×10^{-4}	9.7×10^{-5}	1.6×10^{-4}	1.1×10^{-4}
Reynolds number (-)	$i = 1$	0.7	0.3	0.5	0.3
	$i = 2$	1.2	-	0.9	-
	$i = 5$	-	1.6	-	1.7
	$i = 10$	5.6	3.3	4.5	3.3

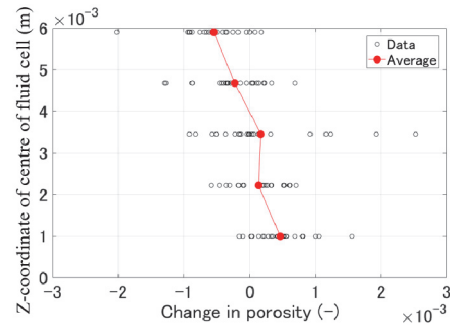
The most plausible explanation for the variation in permeability in all the samples is the variation in porosity in this sample due to seepage as shown in Figure 5.11. Referring to Figure 5.11, in general for all the samples, the change in porosity in the upper fluid cells was negative while there was an increase in porosity in the lower fluid cells. A reduction in porosity should correspond to a reduction in permeability. Initially, a fine particle is sitting on other coarse particles as shown in Figure 5.12 (a). When fluid flow is applied, it seems that these fine particles become suspended in the void with no connectivity (Figure 5.12 (b)). Then, the particle moves upwards and has contacts new coarse particles as illustrated in Figure 5.12 (c), giving a reduction in porosity in the upper layers under fluid flow. As well as the observation of the porosity, the number of fine particles is also observed here as shown in Figure 5.13. As a general trend, the number of fine particles in the upper layer increases, whereas that in the lower layer decreases. Although the number of particles is small except in the G25_Loose sample, more fine particles move upwards for the loose samples. Therefore, the permeability overall will decrease as the simulation proceeds. In addition, the change in porosity at the stable state under $i = 10$ of all the samples is shown in Figure 5.14. These data consider the initial state with no fluid flow relative to the state with $i = 10$. The data in Figure 5.14 show that the magnitude of the change in porosity increases as the hydraulic gradient is incremented above 1.



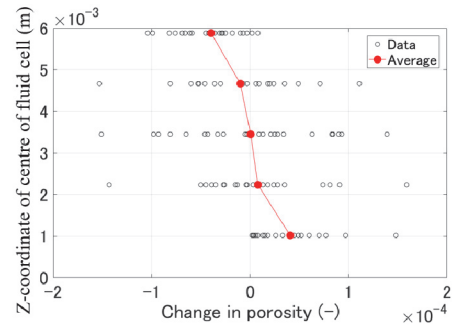
(a) Gap25_Loose



(b) Gap25_Dense

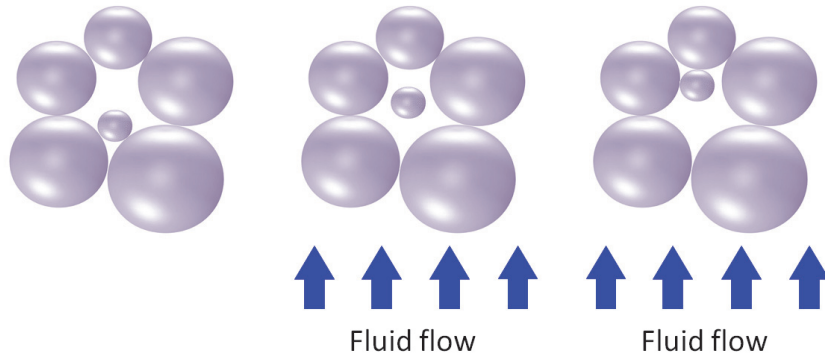


(c) Gap35_Loose



(d) Gap35_Dense

Figure 5.11 Change in porosity of each layer under $i = 1$

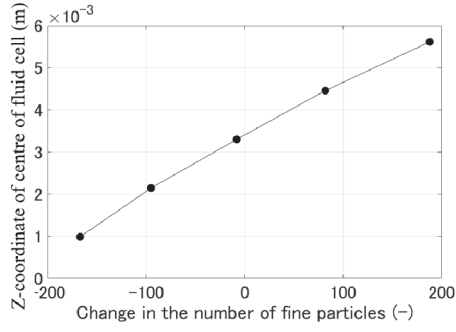


(a) Initial state

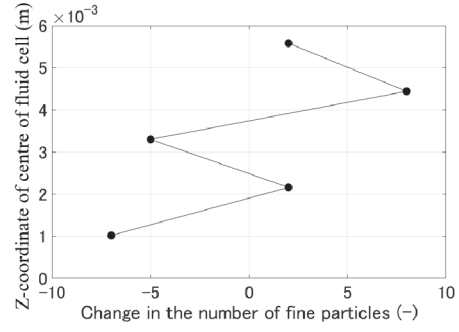
(b) Under fluid flow

(c) Stable state

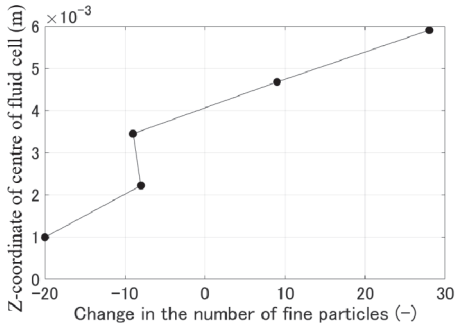
Figure 5.12 Schematic figure of fine particle migration



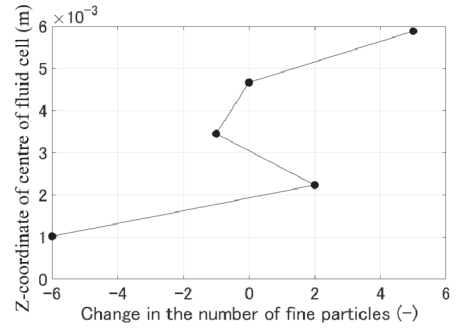
(a) Gap25_Loose



(b) Gap25_Dense

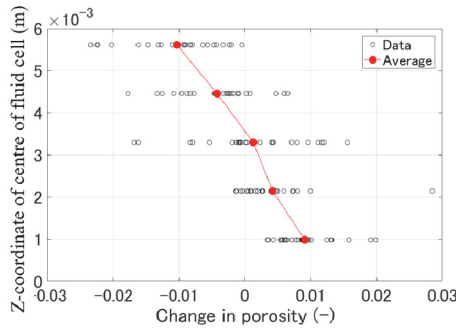


(c) Gap35_Loose

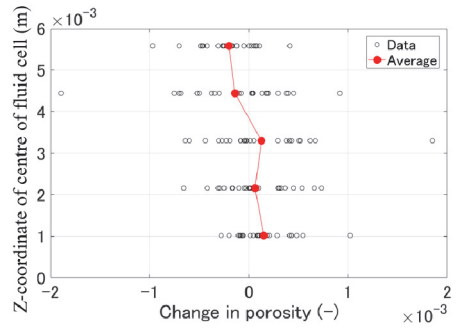


(d) Gap35_Dense

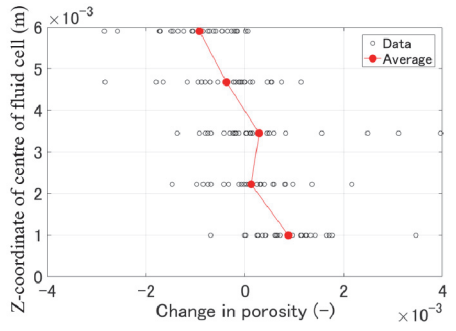
Figure 5.13 Change in number of particles within each layer under $i = 10$



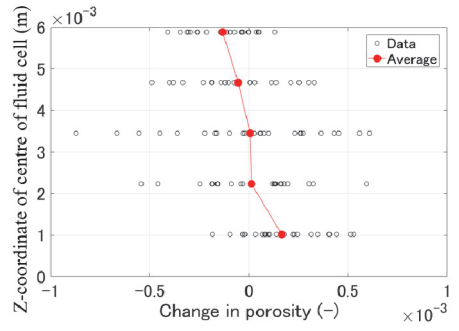
(a) Gap25_Loose



(b) Gap25_Dense



(c) Gap35_Loose



(d) Gap35_Dense

Figure 5.14 Change in porosity of each layer under $i = 10$

The reduction in permeability can be rationally explained by considering the effective permeability of a layered system. For a layered system of the type illustrated in Figure 5.15, the effective permeability is given by:

$$k_{v,eff} = \frac{L}{\sum_1^{n_layers} \frac{L_{n_layers}}{k_{n_layers}}} \quad 5.2$$

where L is the total depth of the soil; L_{n_layers} is the depth of soil in layer n_layers ; and k_{n_layers} is the permeability of layer n_layers . Consider a simple system with two layers, so that $L_1 = L_2 = 0.5L$. The sample is initially homogeneous with a permeability k . If there is a change, so that k_1 increases to $1.1k$ and k_2 reduces to $0.9k$ the effective permeability is:

$$k_{v,eff} = \frac{1}{\frac{0.5}{0.9k} + \frac{0.5}{1.1k}} = \frac{0.99k}{1} \quad 5.3$$

i.e. there is a small net reduction in permeability.

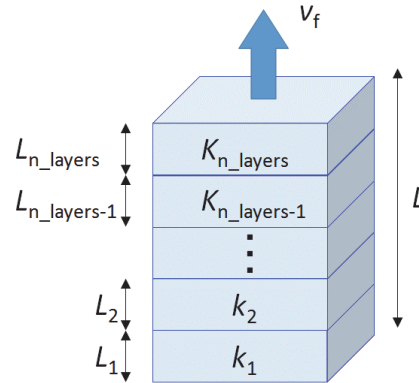


Figure 5.15 Simulated and expected permeability values

Figure 5.16 shows relationship between the discharge velocity and the hydraulic gradient at the stable state. As listed in Table 5.5, the relationship is linear, so fluid flow agrees with Darcy's law. There are only negligible changes in slope as i increases. According to Trussell & Chang (1999), regimes of fluid flow in porous media can be divided into four regimes: Darcy ($Re < 1$), Forcheimer ($Re < 100$), Transition ($Re < 800$) and Turbulent ($Re > 800$). Referring to Trussell & Chang (1999), Darcy flow has no significant inertial contribution and is both laminar and

creeping. In the Forcheimer regime, the flow is also laminar but inertial effects are starting to contribute to the observed stream lines. Although the threshold between Darcy and Forcheimer is $Re = 1$, the relationship between the discharge velocity and the hydraulic gradient of $i < 10$ seems to follow the laminar and creeping flow. Note that the slopes of these lines for all data and each section give permeability values. These are included in Table 5.3 and agree with the stable values obtained by considering a single $v_{\text{discharge}}$ and i value at the stable state when $i = 1$.

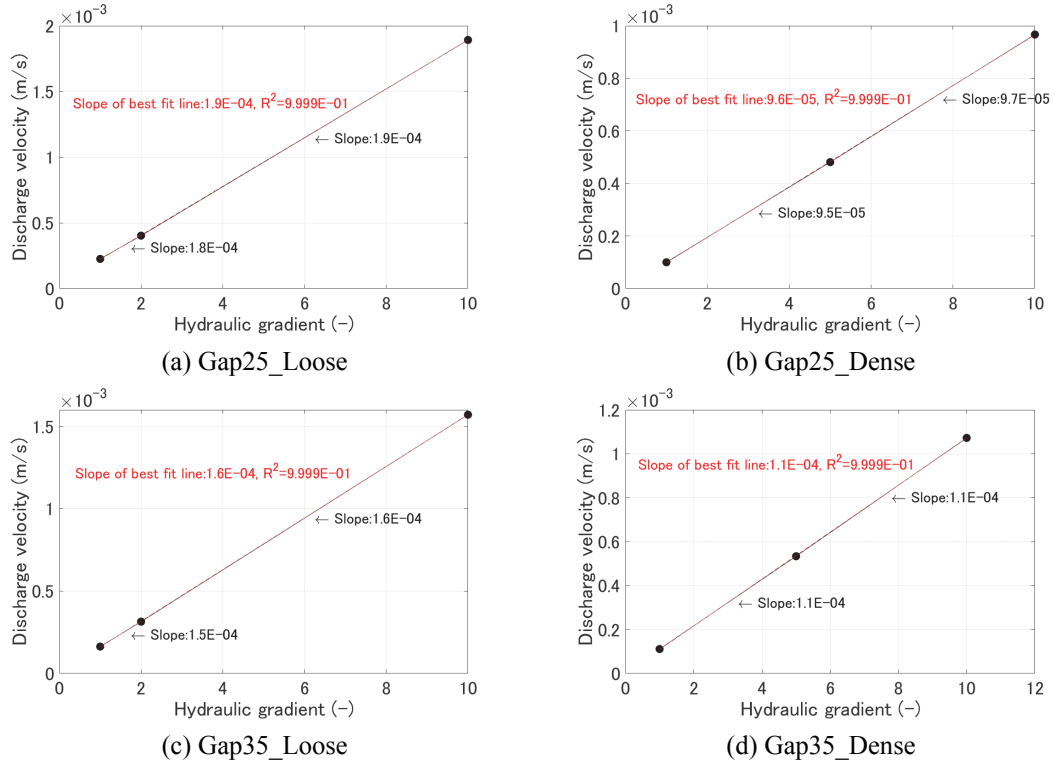


Figure 5.16 Relationship between discharge velocity and hydraulic gradient

Table 5.5 Slope value and Reynolds number under $i > 1$

Sample	Gap25_Loose		Gap25_Dense		Gap35_Loose		Gap35_Dense	
i	1 to 2	2 to 10	1 to 5	5 to 10	1 to 2	2 to 10	1 to 5	5 to 10
Slope	1.8×10^{-4}	1.9×10^{-4}	9.5×10^{-5}	9.7×10^{-5}	1.5×10^{-4}	1.6×10^{-4}	1.1×10^{-4}	1.1×10^{-4}
Re	0.7 to 1.2	1.2 to 5.6	0.3 to 1.6	1.6 to 3.3	0.5 to 0.9	0.9 to 4.5	0.3 to 1.7	1.7 to 3.3

5.3.2. Analysis of normalised particle stress

Following the ideas of Skempton & Brogan (1994) and Shire et al. (2014) as well as the dependency of instability on the stress state observed by Chang et al. (2012), it is important firstly to understand the extent of the stress heterogeneity in each sample. Figure 5.17 gives cumulative distribution functions (CDFs) of normalised particle stress (α_{particle}) values for each sample

following isotropic compression and prior to applying fluid flow. The average stress reduction factor (α, p') values are included in the legend, and the data for equivalent samples considered by Shire (2014) are also considered. The initial α, p' considered in Sections 2.2.3, 2.3.2 and 3.4.3 is the ratio of the mean particle stresses for all fine particles ($\overline{\sigma_{fine}}$) to the overall average stress ($\overline{\sigma_{ij}}$), i.e. $\alpha, p' = \frac{\overline{\sigma_{fine}}}{\overline{\sigma_{ij}}}$; on the other hand, $\alpha_{particle}$ is defined as the normalised particle stress as follows:

$$\alpha_{particle} = \frac{\overline{\sigma_{particle}}}{\overline{\sigma_{ij}}} \quad 5.4$$

where $\overline{\sigma_{particle}}$ is the stress tensor for a given particle as before (Equation 2.9); $\overline{\sigma_{ij}}$ is the (continuum) stress tensor acting throughout volume as before (Equation 2.8).

It is clear that there are a large number of particles (30%) transmitting negligible or very small stresses for the Gap25_Loose sample, which has an overall α value of 0.11. Likewise, Gap35_Loose has 20% of particles transmitting negligible or very small stresses from Figure 5.17. In comparison with the result of Shire et al. (2014), CDFs of the particle stress values except Gap25_Dense are in good agreement with the result considered here. This is probably because the samples with fines contents that are considered transitional are sensitive to the preparation method as illustrated in Figure 2.17.

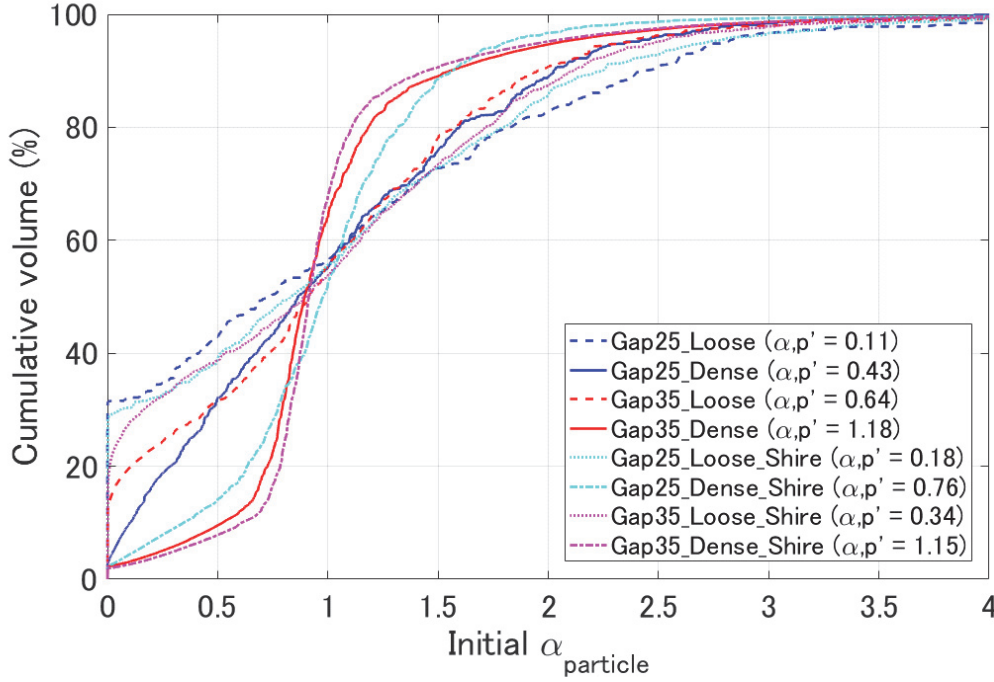


Figure 5.17 CDF for initial α_{particle} in terms of cumulative volume in comparison with the work of Shire et al. (2014)

5.3.3. Analysis of change in coordination number

The change in the coordination number over the whole process is given in Figure 5.18, and the change in the mechanical coordination number is shown in Figure 5.19. After applying water as shown in Figure 5.18 and Figure 5.19, the coordination number abruptly drops since some particles lose connectivity. Following the initial drop in coordination number when fluid flow is applied, in all cases the coordination number then increases gradually and monotonically. This indicates that the particles find new equilibrium positions in contact with other particles as illustrated in Figure 5.12, i.e. they are not simply suspended in the fluid after an initial movement. This is to be expected for the low velocity or low Reynolds number (Equation 4.8) considered here, i.e. clearly laminar and either in the Darcy or Forcheimer regime. After the initial drop, the coordination number gradually increases, and the coordination number gradually converges to a stable value for each applied i . When the increment in coordination number over a time of 0.01 numerical seconds is less than 0.5% as mentioned in Section 5.2.1, the sample is regarded as being stable. The term “stable” is used here to mean that the changes in the sample experiencing under continued flow at this hydraulic gradient are considered to be negligible. There is little difference between the change in the coordination number and change in the mechanical coordination number as each particle in the four samples has connectivity exceeding two referring to Equation 3.3.

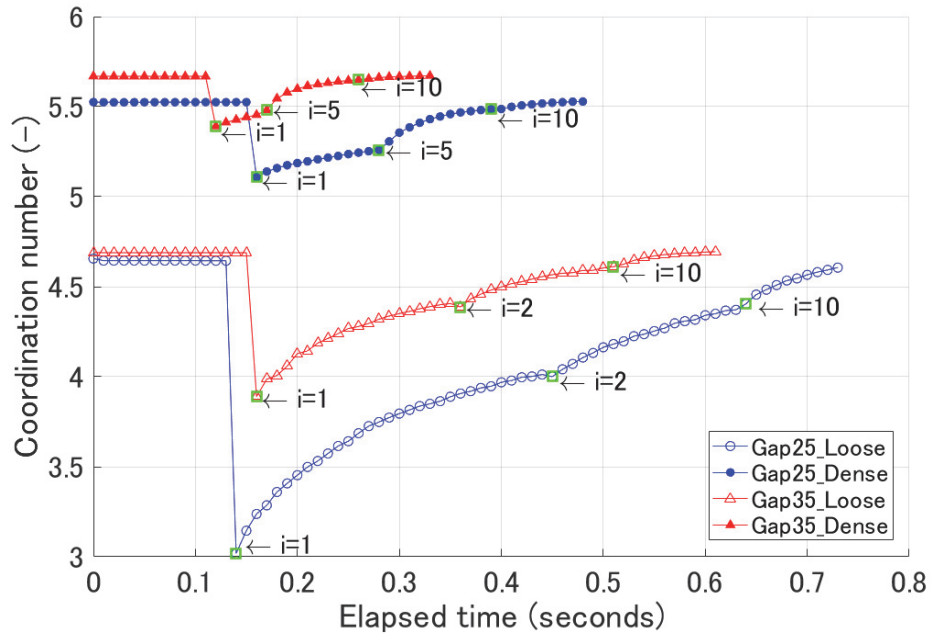


Figure 5.18 Change in coordination number

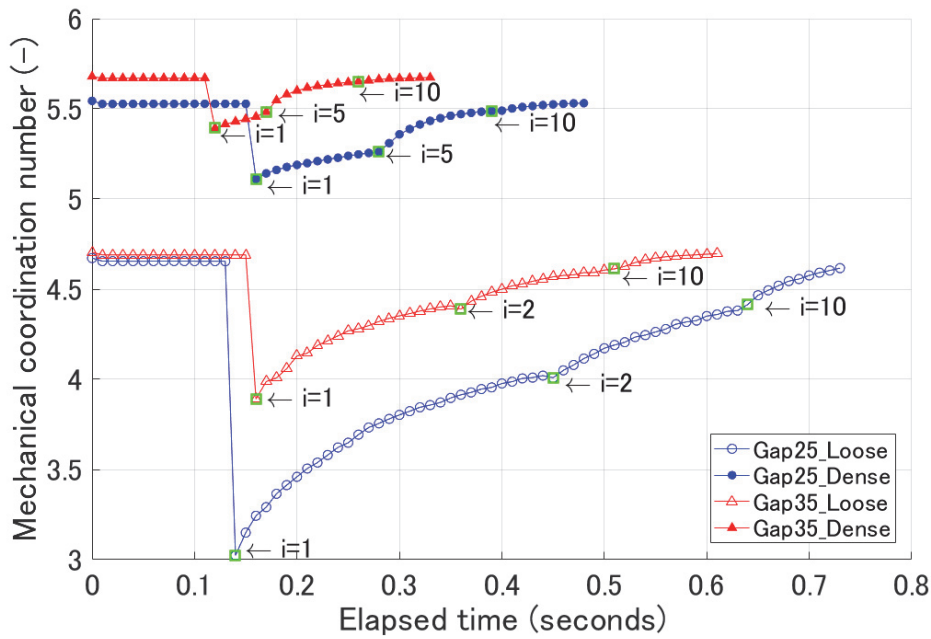


Figure 5.19 Change in mechanical coordination number

The relationship between the initial drop in coordination number ΔZ and the initial average stress distribution in the fines is also summarised in Table 5.6. Figure 5.20 shows the relationship between the initial drop of coordination number (Z) and the initial α_p . The sample

with the lowest initial α, p' (Gap25_Loose) had the largest drop in coordination number, while the sample with the highest initial α, p' (Gap35_Dense) had the smallest initial drop in coordination number.

Table 5.6 Hydro-mechanical properties obtained from simulations under $i = 1$

Hydro-mechanical property		Gap25_Loose	Gap25_Dense	Gap35_Loose	Gap35_Dense
Average stress reduction factor, α, p'		0.11	0.43	0.64	1.18
Porosity, n		0.268	0.237	0.278	0.257
Permeability (m/s)		2.3×10^{-4}	1.0×10^{-4}	1.6×10^{-4}	1.1×10^{-4}
Reynold number, Re		0.7	0.3	0.5	0.3
Initial drop of Z		1.63	0.42	0.80	0.28
Initial drop of Z_{mech}		1.66	0.42	0.80	0.28
Average velocity (m/s)	Discharge	2.3×10^{-4}	1.0×10^{-4}	1.6×10^{-4}	1.1×10^{-4}
	Seepage	8.4×10^{-4}	4.2×10^{-4}	5.9×10^{-4}	4.3×10^{-4}
Displacement (m)	Max	1.6×10^{-4}	2.3×10^{-5}	5.3×10^{-5}	1.0×10^{-5}
	Average	3.9×10^{-5}	8.0×10^{-7}	3.3×10^{-6}	2.6×10^{-7}
	Median	3.6×10^{-5}	1.0×10^{-9}	4.1×10^{-8}	0.0

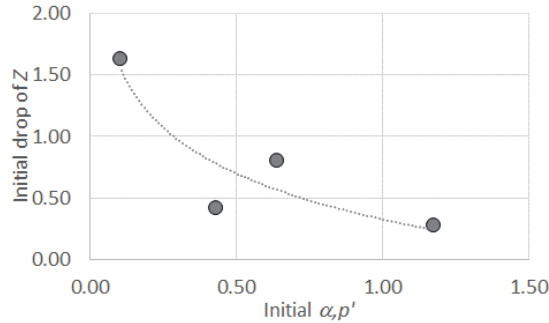


Figure 5.20 Influence of initial α, p' to initial drop of Z

5.3.4. Particle migration

In this study, particle migration is used to identify the onset of suffusion. In order to determine what percentage of particles move due to seepage flow, the particle displacements were calculated using Equation 5.1. It is important to acknowledge that the magnitude of the displacement is strongly related to how much stress particles transfer and how long particles are under seepage flow. The displacement values given here were extracted when the coordination number was stable. The displacement of all particles in the four samples are widely distributed as can be seen by considering the cumulative distribution function (CDF) plots of the data in Figure 5.21. In Figure 5.21, the particle migration limit is shown as well, meaning that particles can

theoretically move up to this upper limit. The particle migration limit is calculated by the seepage velocity times the simulation time.

Comparing the four samples, in the first instance, there is obviously a density effect. The shape of the CDFs differ for the loose and dense packings. In the dense samples, many particles effectively remained stationary, while there was a broader range of displacement values for the loose samples. Both the average and maximum displacements were higher in Gap25_Loose, compared with Gap35_Loose. This can be related to the α, p' values ($\alpha_{\text{Gap25_Loose}} < \alpha_{\text{Gap35_Loose}}$), and the shape of the CDF of the initial α_{particle} before applying water as shown in Figure 5.17; there are more unstressed particles in Gap25_Loose in comparison with Gap35_Loose. For the dense packings in Figure 5.21, both samples have similar behaviour, i.e. the majority of particles moved less than 1.0×10^{-8} m. There was insufficient void space to allow particles in the dense samples to move, and the α, p' values were high enough that fines were confined under stress. Interestingly, $\alpha_{\text{Gap25_Dense}}$ is smaller than $\alpha_{\text{Gap35_Loose}}$, however, there were more stationary particles in Gap25_Dense. The initial α, p' is probably not only the factor determining whether particle migration occurs. The initial coordination number is higher in Gap25_Dense when compared with Gap35_Loose.

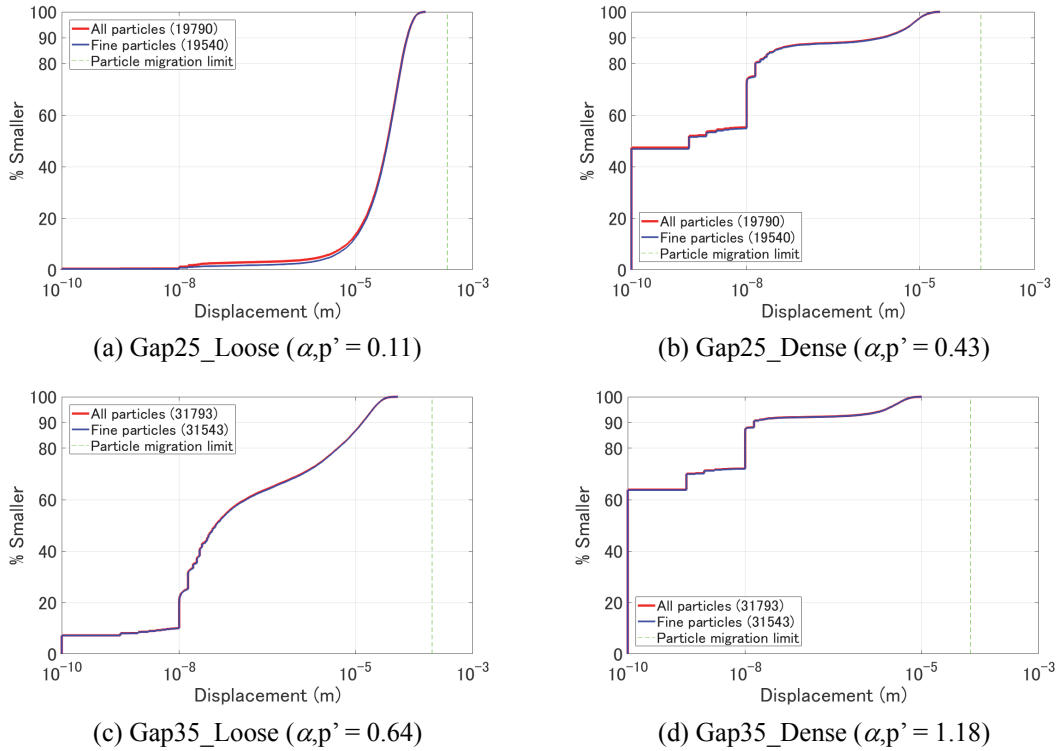


Figure 5.21 CDF for all particle displacement under $i = 1$ (Note that the number in round bracket is the number of particles)

It is difficult to assess from the raw CDF plots whether the displacements observed indicate erosion is occurring. Figure 5.22 uses histograms to assess the link between displacement and the change in contact conditions. The histogram gives the number of particles experiencing a given range of displacement values. Then, for each histogram bin, the displacement values of each particle are given as a data point, and the average displacement was also calculated. Considering the data in Figure 5.22, a large number of particles do not have any change in connectivity, and the particles with zero change in connectivity have the least average displacement for samples of Gap25_Dense, Gap35_Loose and Gap35_Dense. However, it is possible that a group of particles might move together as a cluster or clump under seepage load or a particle could move from one position to another with the same connectivity. A reduction of the connectivity tends to induce the biggest displacement. Particles with low displacement are more likely to have an increase in connectivity. These likely include particles at rest which gain contacts as other particles move into contact with them.

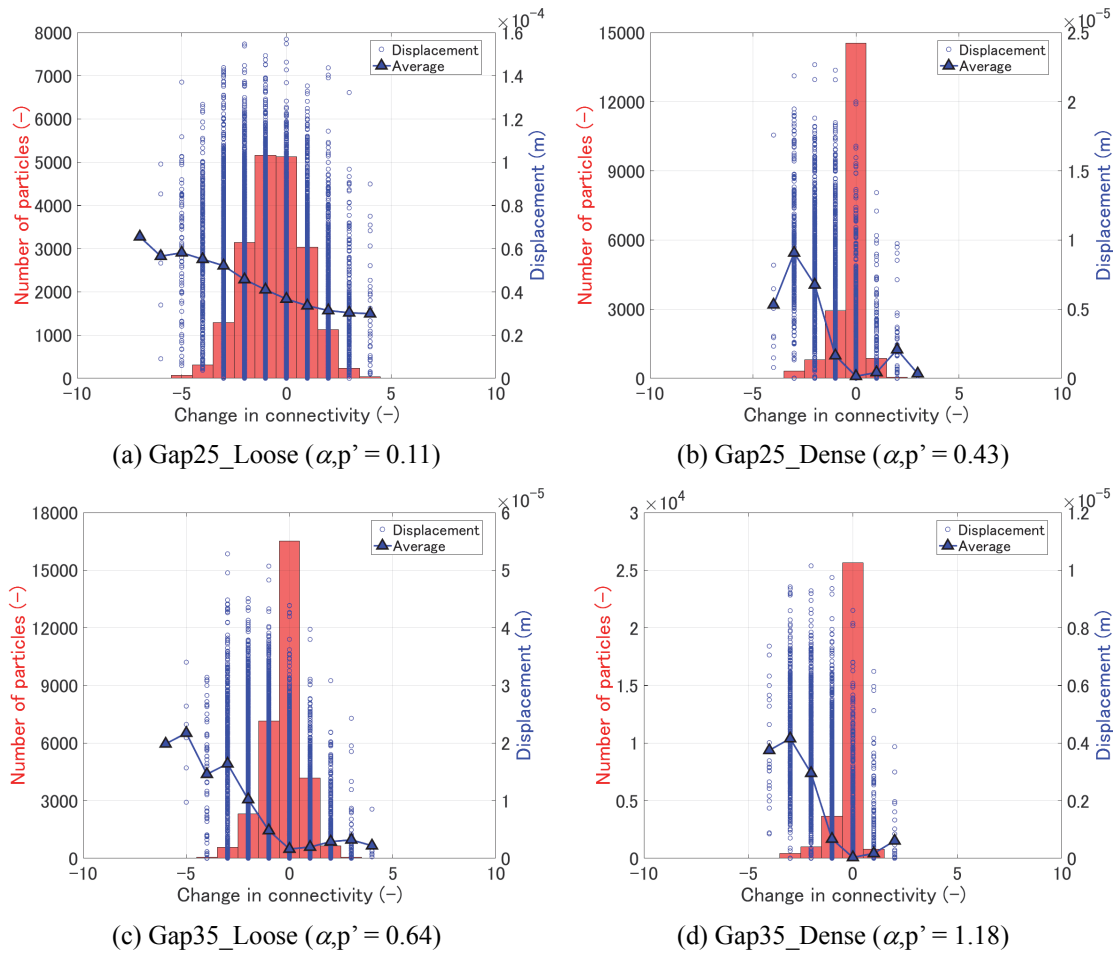


Figure 5.22 Relationship between change in connectivity and fine particles displacement under $i = 1$

The magnitude of the particle displacement is taken here to be an index indicating whether particle erosion has occurred. Focussing on the relationship between particle displacement and initial α_{particle} as shown in Figure 5.23, there is a distinctive trend that particles with low initial α_{particle} are inclined to have a large displacement, i.e. the less constrained particles move further if there is a sufficient space. As shown in Figure 2.17, samples with approximately $0.4 < \alpha_{\text{p}'} < 0.8$ are sensitive to stress applied. The data are widely scattered in the Gap25_Dense sample. On the other hand, the data for other samples are clearly divided into the two fields: large particle displacements associated with a low initial α_{particle} and small particle displacements associated with a large initial α_{particle} . The data in Figure 5.24 indicate the same trend. In Figure 5.24, a histogram shows the number of particles associated with specific intervals of α_{particle} values and the average displacement associated with each interval. In the Gap35_Loose sample, the initial α_{particle} values are widely spread. For the loose samples, the average displacement increases in the highest α_{particle} values, there is no significance for this increment as it is associated with very few particles. However, most particles have low initial α_{particle} for the Gap25_Loose sample, and most particles with large initial α_{particle} for the Gap25_Dense and Gap35_Dense are confirmed in Figure 5.24. In general, it is clearly found that particles with low initial α_{particle} are responsible for the most of the particle migration.

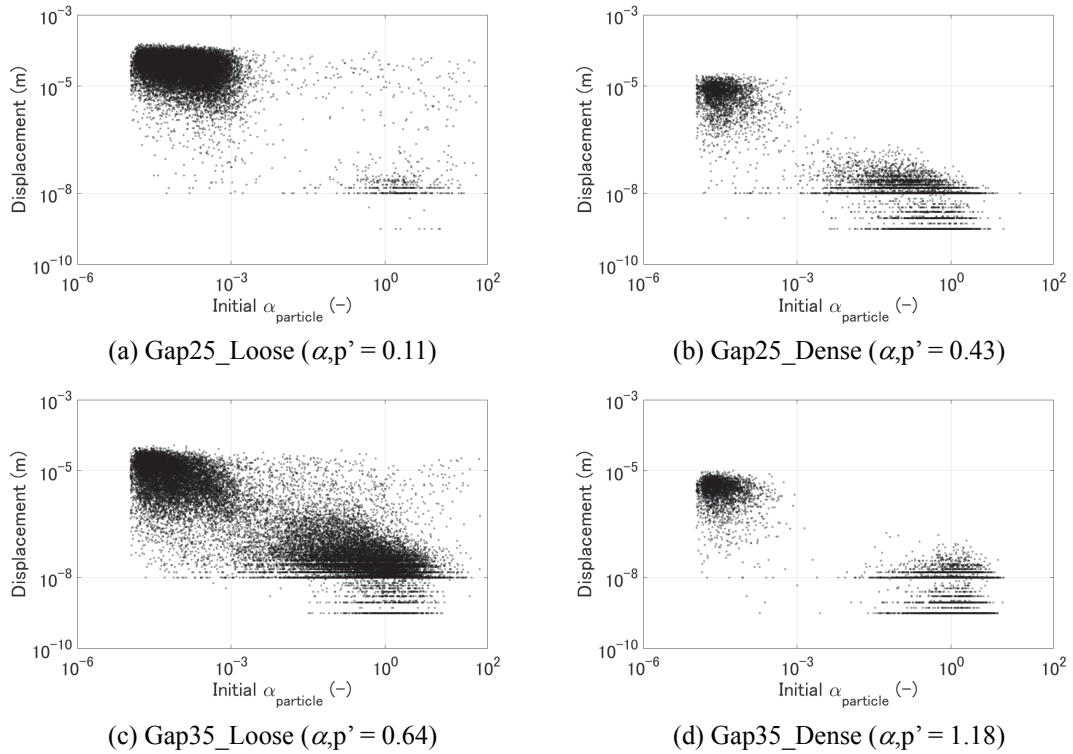


Figure 5.23 Relationship between initial α_{particle} and all particles displacement under $i = 1$

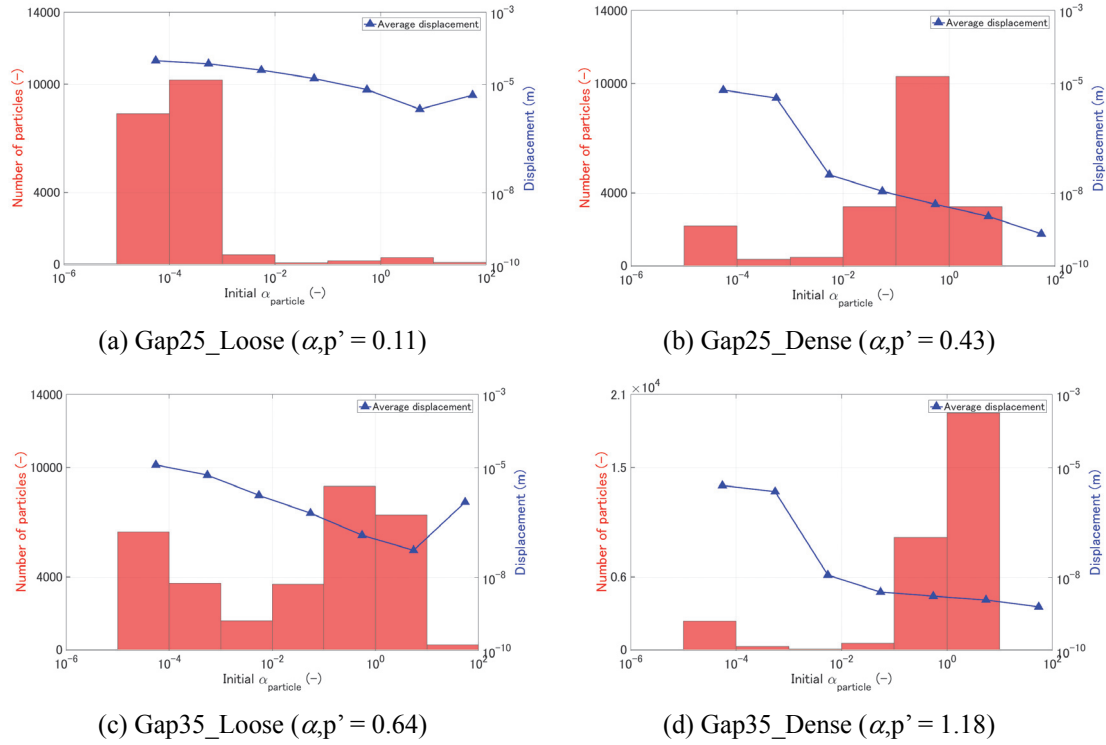


Figure 5.24 Histogram of initial α_{particle} and average all particles displacement under $i = 1$

5.3.5. Influence of seepage velocity

As mentioned in Section 2.2.1, seepage velocity (Equations 2.1 to 2.3) flowing through each fluid cell is possibly a key factor for suffusion. The effect of seepage velocity is considered here. The relationship between particle displacement and seepage velocity is shown in Figure 5.25. Note that the seepage velocity for a particle is the seepage velocity for the fluid cell in which the particle has its centroid. Note that there is a variation in seepage velocity amongst the fluid cells due to sample heterogeneity. It is clearly shown that displacement increases with increasing seepage velocity in all four samples since the drag force is also increased with seepage velocity. Seepage velocity increased in proportion to the magnitude of hydraulic gradients. Considering the terminal velocity (Equation 4.14), all particles experience a seepage velocity that exceeds their respective terminal velocities as given in Figure 5.26, meaning that all particles can move some distance in the absence of applied forces including contact forces. The relationship between both seepage velocity and the initial normalised particle stress (α_{particle}) values and the particle displacement is considered as given in Figure 5.27. As a general trend, displacement clearly becomes larger with the reduction in α_{particle} value and the increment in seepage velocity as mentioned in the previous section. In addition, it is clear that the particles with $C_{\text{particle}} \geq 4$ appear to have small overall displacements and have the bigger initial α_{particle} values as mentioned in Section 5.2.2.

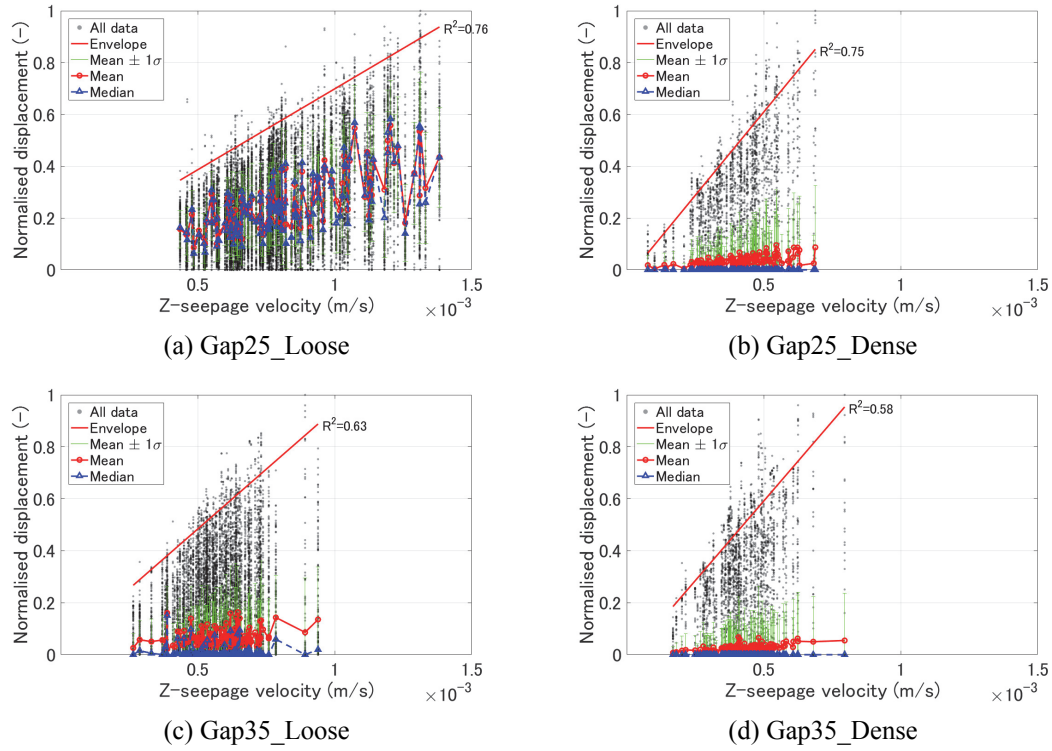


Figure 5.25 Relationship between fine particles displacement and seepage velocity under $i = 1$ (Note that all displacement values are divided by the maximum displacement value)

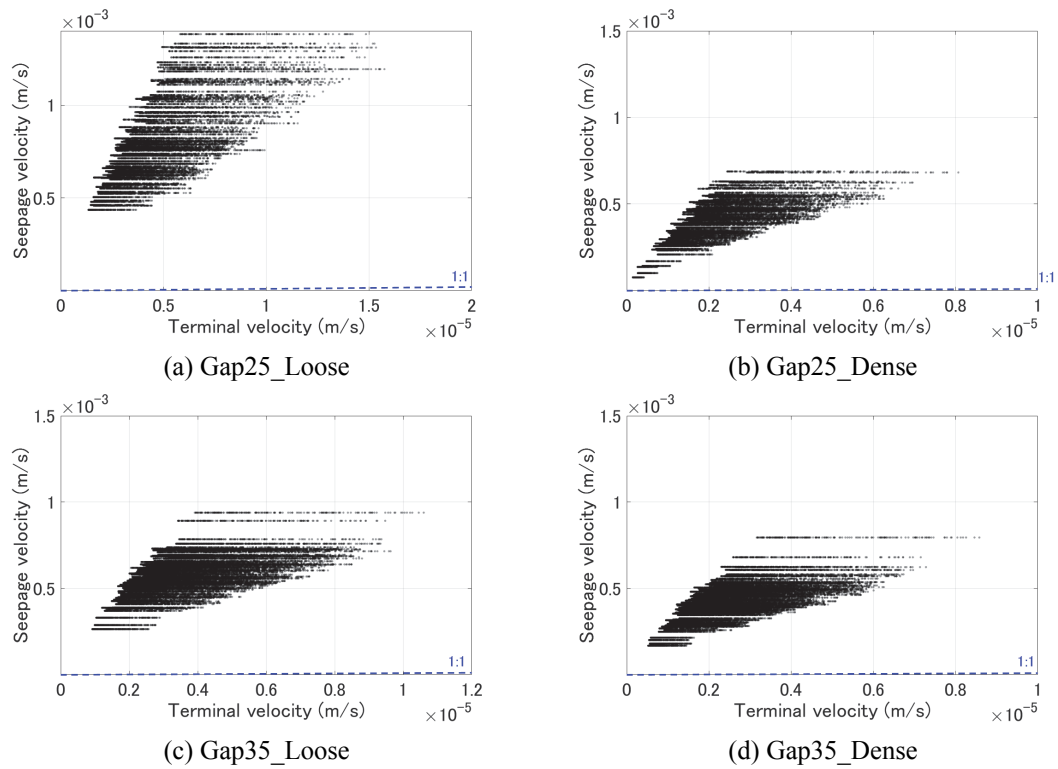


Figure 5.26 Relationship between seepage and terminal velocity under $i = 1$

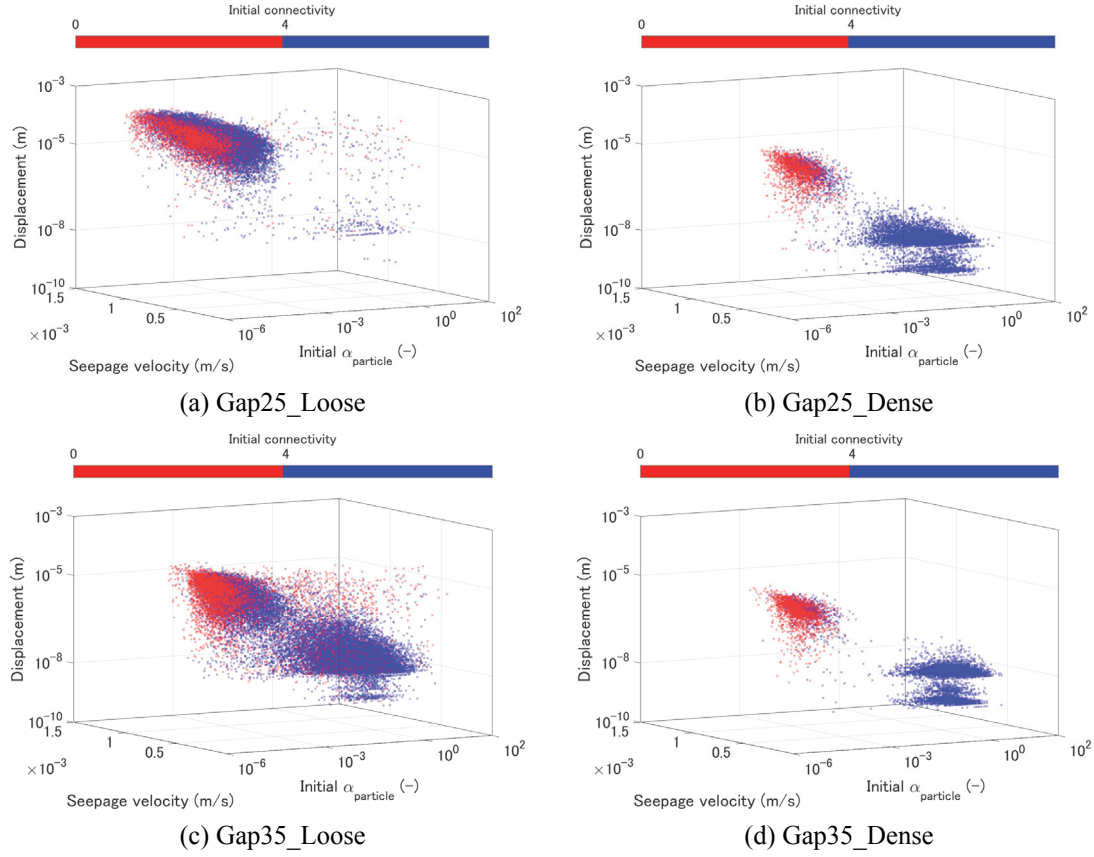


Figure 5.27 Relationship between fine particles displacement, initial α_{particle} and seepage velocity under $i = 1$

5.4. Conclusions

This chapter has examined the susceptibility of four different samples to internal instability by considering the results of DEM simulations of four different virtual permeameter tests. The analyses considered the permeability, the seepage velocity, the initial normalised particle stress (α_{particle}), the coordination number (Z), the mechanical coordination number (Z_{mech}), the connectivity (C_{particle}) and the particle displacements.

In terms of permeability, the simulated values are in good agreement with the empirical and experimental values. In particular, the values from the Hazen equation are almost the same as the simulation values, whereas the values from the Chapius equation indicate the lowest permeability values. These equations use D_{10} . For the Gap35_Loose sample, there is good agreement with the experimental data from the work of Slangen (2015). The simulation data were within an order of magnitude of the values predicted using the Di Felice and the Ergun equations. These expressions use D_{50} . Overall, the simulated permeability can be regarded as being reasonable although the appropriateness of using expressions based on D_{50} of gap-graded

soil needs to be considered. The velocity was proportional to the hydraulic gradient (i) in accordance with Darcy's law.

It is shown that there is sudden drop of the coordination number (Z) and mechanical coordination number (Z_{mech}) and an increase in the seepage velocity when i is applied to the samples. Z and Z_{mech} increase until a stable state is achieved, where “stable” means that the change in Z and Z_{mech} is negligible. Considering the influence of the initial α_p , the initial drop of Z and Z_{mech} are strongly linked to the initial α_p . The intensity of initial drop in coordination number decreases as α_p increases.

Chapter 6. CONCLUSIONS

6.1. Summary

The aim of the research described here was to apply coupled DEM-CFD modelling to simulate permeameter tests with a constant head on gap-graded materials to improve our understanding of mechanisms that govern the onset of suffusion at the particle scale. Material susceptibility has been considered in prior particle-scale research (Shire, 2014); however, the hydro-mechanical aspects of susceptibility at the particle scale have received little prior consideration. The coupled DEM-CFD simulation approach used here contributes to identifying factors associated with particle migration caused by suffusion.

As mentioned in Chapter 2, understanding the mechanism of suffusion is essential for safety evaluation of internal erosion; three categories of factors that govern the onset of suffusion are given as material, hydraulic and mechanical susceptibility as illustrated in Figure 1.1. However, identifying the initiating mechanism is not straightforward. Many researchers have reported that internal erosion was occurred at much lower hydraulic gradient than the critical hydraulic gradient obtained from Terzaghi's theory. Perhaps, the most important contribution in this discussion was the work of Skempton & Brogan (1994). More recently, Moffat & Fannin (2011) and Chang & Zhang (2013) investigated the relationship between hydraulic gradients and stress. The experimental results showed that increase in stress linearly caused the increase of a hydraulic gradient. In addition, Skempton & Brogan (1994) defined stress reduction factor (α) to explain the susceptibility to internal erosion. Muir Wood et al. (2010) and Maeda et al. (2012) studied suffusion using DEM; however, they did not consider the onset of suffusion. Some researchers have started to observe internal erosion using DEM-CFD to determine which parameters are responsible for particle migration. Even though strong proof regarding the initiation of suffusion is not confirmed yet, some progress has been made. Most notably, Farahnak Langroudi et al. (2013) and Shire (2014) developed the idea of α , and Shire (2014) found that α was strongly linked to fines content.

DEM samples were developed in Chapter 3. The influence of preparation method, density and the number of particles was observed. Two methods were used to prepare samples in DEM: compression and pluviation. Considering inhomogeneity, the variability in porosity was significant in smaller samples, and the variability in porosity in the pluviated samples was higher than that in the compressed samples. In particular, the porosity near the rigid walls was higher than in the other layers. The dense samples had low porosities and large coordination numbers

when compared with the loose samples. With respect to α , the loose samples generally had smaller α values than the dense samples, and these results are in good agreement with those of Shire (2014). So as to avoid inhomogeneity near rigid walls, a measurement sphere was used to analyse α . The general trend was that α within the measurement sphere was low in comparison with that in overall sample. Fabric anisotropy was also quantified. There was no significant anisotropy in the compressed samples, whereas the pluviated samples showed some anisotropy.

In Chapter 4, the simulation of particle-fluid interaction was discussed considering the Navier-Stokes equations and the coarse grid method. Before the coupled DEM-CFD code was used, limitations associated with code validation were identified. The study highlighted the need for users to validate codes or software themselves even where commercially developed packages are used. For simple validation, a terminal velocity of one particle was theoretically calculated using the Newton's second law, which agreed with values from simulation. Following the simple validation, the work of Suzuki et al. (2007) was considered as a case with multiple particles. Following some corrective steps taken by the software developers, the results obtained from the coupled DEM-CFD code were similar to theoretical values, meaning that the coupled DEM-CFD code was successfully validated using analytical solution.

The virtual permeameter test simulations were carried out in Chapter 5. Four samples with two fines contents and two densities were used. Permeability values from simulation were compared with both empirical and experimental values in a validation or verification step. Four empirical equations were used, and the discrepancy between the simulated and expected values was within one order of magnitude. In particular, the Hazen equation had the best agreement with the simulated values. The discharge velocity was proportional to the hydraulic gradient, so fluid flow was clearly regarded as following Darcy's law. When a hydraulic gradient was applied to the samples, the coordination number (Z) abruptly dropped and then gradually increased until Z stabilised. The initial drop of Z was related to the initial stress reduction factor (α_p) calculated from the average mean normal stress. Particle displacement decreased with increasing of α_p , and decreasing seepage velocity. Considering the initial normalised particles stress (α_{particle}), some mobile particles had large α_{particle} , hence the change in mean normal stress contributed to the migration of these particles.

6.2. Key findings

Following the introduction (Chapter 1) and the literature review (Chapter 2), the contributions to new understanding made in this study are given in Chapter 3 to Chapter 5. The key findings in terms of sample evaluation in Chapter 3 are:

- Large porosity near rigid walls causes inhomogeneity, especially in both ends of samples due to the relatively large diameters.
- The α values from simulation are in good agreement with the results from the work of Shire (2014).
- The stress reduction factor (α) of the small sample is higher than that of large samples.
- The samples with 35% fines content have larger α , i.e. fine particles transfer much stress in comparison with the samples with 25% fines content.
- The variation in α in pluviated samples is larger than that in compressed samples.
- There is no significant fabric anisotropy under isotropic compression, whereas some fabric anisotropy with pluviated method is confirmed.

The key findings from the work presented in Chapter 4 are:

- The settlement and pore water pressure are successfully validated in comparison with theoretical values in the work of Suzuki et al. (2007).
- It is important to check continuity to validate the coupled DEM-CFD code even though it is commercial software.
- Large models have less numerical oscillation than small models when the hydraulic gradient is initially applied using the coarse-grid approach.

The key findings in terms of particle migration due to suffusion in Chapter 5 are:

- Permeability values from the simulations are in good agreement with empirical values, especially for the Hazen equation.
- The permeability value from simulation for Gap35_Loose is almost the same as experimental data for an equivalent from the University of British Columbia.
- Discharge velocity increases in proportion to hydraulic gradient, implying in that fluid flow is laminar.
- There is sufficient space in the voids to allow fine particles to migrate within the void space.
- The coordination number abruptly drops, and seepage velocity increases when a hydraulic gradient is applied. Then, coordination number increases until fluid state is deemed stable.
- The particle displacement increases as the magnitude of change in connectivity reduces.
- The initial drop of coordination number (ΔZ) is influenced by initial normalised particle stress (α_{particle}), generally ΔZ increases as α_{particle} reduces.
- Particle displacement increases as α_{particle} decreases.
- Seepage velocity always exceeds terminal velocity of particles under $i > 1$.
- Seepage velocity linearly affects maximum particle displacement.

6.3. Recommendations for future work

This research has not been exhaustive, and findings described in previous section can be developed in future research. A critical limitation of using the coupled PFC3D-CCFD code is that the coupled numerical analysis is highly time-consuming. This limits the size of sample, the range of particle sizes and the complexity of the scenarios modelled. Recommendations for further study are shown below.

The samples considered have only a D'_{15}/d'_{85} of 4.6 of the Kezdi criterion. It means that these samples are internally unstable, so the samples are regarded as being susceptible to internal erosion. However, 4.6 is close to the threshold of 4.0, meaning that a sample with 4.0 of the Kezdi criterion is stable. Further insight would be gained by looking at samples with a broader range of D'_{15}/d'_{85} values. In particular, samples considered by Shire (2014) and Skempton & Brogan (1994) should be considered.

Although coupled DEM-CFD analyses are computationally expensive, it is important to continue to use this modelling approach. Some researchers use open source codes such as LIGGGHTS, OpenFOAM or YADE-OpenFOAM. These codes are Linux-based, so high performance computers or super computers can be used with these codes. The advantage of this is that time can be significantly saved, and the number of particles can be increased.

In this thesis, the maximum hydraulic gradient considered is 10; however, $i = 20$ can be applied to the samples under laminar flow according to Mitchell & Soga (2005). For instance, in the work of Moffat et al. (2011), up to $i = 30$ was applied to a sample under isotropic compression of 50 kPa. It would be interesting to consider these cases.

A large number of numerical analyses may be interested in the effect of fluid cell size. Following the recommendation from Itasca, at least five particle diameters should be placed in along one fluid cell length. According to the validation of Suzuki et al. (2007), this recommendation was breached. In spite of the violation, the values from the coupled DEM-CFD were good in agreement with the theoretical values and the values from the work of Suzuki et al. (2007). Investigating the effect of the fluid cell size would be useful.

Finally, the coupled DEM-CFD uses the coarse grid method proposed by Tsuji et al. (1993). The disadvantage of using this method is that the detailed information around one particle cannot be monitored, i.e. only representative values can be collected. This is efficient enough for practical problems although it takes a long time to finish simulations. However, one of the key

factors dominating suffusion should be seepage velocity, which is not real fluid velocity flowing through void spaces as shown in the work of Taylor (2016). If fluid mesh is much smaller than the particles, the real seepage velocity can be calculated, leading that real particle-fluid interaction force can be numerically obtained. Fortunately, Mr. Christopher Knight is implementing the Immersed Boundary Method (IBM) to understand the mechanisms of suffusion. This method can solve the Navier-Stokes equations for fluid flow around one particle immersed in the flow field. Thus, IBM can investigate microscopic pore fluid flow to improve understanding of the particle-fluid drag force in porous media at the particle scale.

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Appendix A: User defined function for boundary conditions

The code of the user defined function developed by Jason Furtney at Itasca, which mentioned in Section 5.2.1, is given as:

```
#include <windows.h>
#include <cmath>
#include <string>
#include <fstream>
#include <sstream>
#include "CFDPlugin.h"
#include "getData.h"
#define DLL_BOUND_DATA( func_name ) extern "C" double __declspec(dllexport)
(func_name)(CGetData &data,const int &iCell,const int &iSurf); double __declspec(dllexport)
(func_name)(CGetData &data,const int &iCell,const int &iSurf)
using namespace CRC_CFD;
double error(const char *msg) {
    int msgboxID = MessageBox(
        NULL,
        msg,
        "Error in CCFD user defined boundary condition function",
        MB_ICONWARNING | MB_OK | MB_DEFBUTTON2
    );
    return 0.0;
}

DLL_BOUND_DATA( user_bc_f1 )
{
    std::ifstream infile("user_bc_f1.txt");
    if (!infile.good()) return error("could not open file user_bc_f1.txt¥n");
    std::vector<double> time_list;
    std::vector<double> value_list;
    double value=0;
    std::string line;
    while (getline(infile, line))
    {
```

```

std::istringstream iss(line);
double a, b;
if (!(iss >> a >> b)) { return error("File format error."); }
time_list.push_back(a);
value_list.push_back(b);
}

if (time_list.size() == 0 ||
    (time_list.size() != value_list.size())) return error("Too few lines or bad format.");
if (time_list.size() < 2) return error("Boundary condition data should have at least two
lines.");
if (!time_list[0] == 0.0) return error("The first time value must be zero.");
for (unsigned int i=0; i<time_list.size()-1; i++)
{
    if (time_list[i] > time_list[i+1]) return error("Boundary condition time data must increase
monotonically.");
}

double time = data.getTime();
if (time < 0) return error("internal error, time should not be less than zero");
if (time >= time_list[time_list.size()-1]) return value_list[value_list.size()-1];
for (unsigned int i=0; i<time_list.size()-1; i++)
{
    if ((time >= time_list[i]) && (time < time_list[i+1])) {
        double t0 = time_list[i];
        double t1 = time_list[i+1];
        double v0 = value_list[i];
        double v1 = value_list[i+1];
        double dt = t1-t0;
        double dv = v1-v0;
        return dv*((time - t0)/dt) + v0;
    }
}
return error("internal error, reached unreachable code?");
}

```