Towards Realistic Simulation of Penetration Tests and Instability Analysis of Sand: A Micromechanical Perspective

Seyedshayan Hashemi, The University of Western Ontario

Supervisor: Sadrekarimi, Abouzar, The University of Western Ontario
A thesis submitted in partial fulfillment of the requirements for the Master of Engineering Science degree in Civil and Environmental Engineering
© Seyedshayan Hashemi 2021

Follow this and additional works at: https://ir.lib.uwo.ca/etd

Recommended Citation

This Dissertation/Thesis is brought to you for free and open access by Scholarship@Western. It has been accepted for inclusion in Electronic Thesis and Dissertation Repository by an authorized administrator of Scholarship@Western. For more information, please contact wlsadmin@uwo.ca.
Abstract

In this series of studies, the capability of Discrete Element Method (DEM) to simulate the behavior of granular materials has been examined. In the first study, various boundary conditions are simulated through a series of DEM-based miniature calibration chamber tests to investigate the influence of boundary conditions on cone tip ($q_c$) and sleeve frictional ($f_s$) resistances. The second study focuses on the influence of microparameters such as state, modulus, rolling resistance, inter-particle friction, and probe properties on CPT measurements in a centrifuge setting. DEM has been used in the last study to investigate the instability of granular materials under drained and undrained failure conditions. 3D assemblies of the stacked-ring simple shear device were modeled to simulate monotonic constant volume, constant stress, and drained constant shear stress paths. Overall, DEM can successfully capture the instability and large deformation behavior of granular materials.

Keywords

Discrete Element Method, cone penetration test, boundary condition, microparameters, instability, critical state, granular matter
Summary for Lay Audience

The mechanical behavior of granular materials is predominantly dominated by the forces transmitted through contacts between grains. Simulation of the distinct behavior of soils using continuum approximations has always faced challenges, specifically in modeling large deformation failures. Discrete Element Method (DEM) with a distinct nature can perfectly capture the behavior of granular systems and assemblies by modeling contacts between rigid spheres or disks. Within the confines of this study, DEM has been used to model the behavior of compressible sandy soils. In the first series of this study, a penetration test commonly known as the Cone Penetration Test (CPT) has been simulated. Despite the versatility and simplicity of this test, the application of CPT in remote areas is expensive and requires extensive knowledge of the effect of various parameters in measurements. For this reason, miniature calibration chamber tests have been proposed in the laboratory settings to replicate the penetration tests in a smaller volume of soils. This has led to significant boundary condition problems in the measurements; therefore, various boundary conditions in a miniature cone penetration test has been simulated to capture the actual penetration resistance representing the free-field condition. To illuminate the governing factors in CPT measurements, a series of sensitivity tests have been carried out to investigate the effect of micro and macro parameters on CPT measurements. In the last series of simulations, Direct simple shear test has been simulated as an invaluable test in replicating the static or dynamic liquefaction behavior of sand. Liquefaction is a catastrophic phenomenon occurring in saturated sandy materials, that leads to loss of strength in the medium with the soil behaving as a liquid. This form of instability in granular soils has been fully investigated in the last chapter to understand the failure mechanism in undrained and drained conditions.
Co-Authorship Statement

This thesis has been prepared in accordance with an Integrated-Article format thesis stipulated by the School of Graduate and Postdoctoral Studies at the University of Western Ontario and has been co-authored as:

**Chapter 2: DEM and Experimental Study on the Effect of Boundary Condition on CPT calibration chamber tests**

All numerical work was completed by Seyedshayan Hashemi under the supervision of Dr. Abouzar Sadrekarimi. All experimental work was completed by Ronit Ganguly under the supervision of Dr. Abouzar Sadrekarimi. A paper co-authored by Seyedshayan Hashemi, Ronit Ganguly and Abouzar Sadrekarimi will be submitted to the Canadian Geotechnical Journal.

**Chapter 3: Comprehensive study on the Effect of Microparameters on CPT Measurements**

All numerical work was completed by Seyedshayan Hashemi under the supervision of Dr. Abouzar Sadrekarimi. A paper co-authored by Seyedshayan Hashemi and Abouzar Sadrekarimi will be submitted to the Canadian Geotechnical Journal.

**Chapter 4: Instability of Granular Materials Under Simple Shear Failure Mode: A DEM Perspective**

All numerical work was completed by Seyedshayan Hashemi under the supervision of Dr. Abouzar Sadrekarimi. A paper co-authored by Seyedshayan Hashemi and Abouzar Sadrekarimi will be submitted to the Computer and Geotechnics Journal.
Acknowledgments

First and foremost, I would like to thank my supervisor, Dr. Abouzar Sadrekarimi, for his consistent guidance, support and assistance throughout the progress of this research and methodology.

I would like to acknowledge the support of Itasca consulting group, by providing the license for commercial software Particle Flow Code (PFC) under the Itasca Educational program.

In addition, I would like to thank my parents for their wise counsel and empathetic ear. Finally, an extended thanks to my friends and colleagues, Amirreza and Samira, Armin, Behrad, Ehsan, iHamed, Hamed, Koosha and Hani, Ronit and Arjama, Sadegh, and Neda especially, who supported me in times of need and tough decisions.
# Table of Contents

Abstract ................................................................................................................................. ii
Summary for Lay Audience .................................................................................................... iii
Co-Authorship Statement ....................................................................................................... iv
Acknowledgments .................................................................................................................. v
Table of Contents .................................................................................................................. vi
List of Tables ........................................................................................................................ ix
List of Figures ........................................................................................................................ x
List of Appendices ................................................................................................................ xx
Nomenclature ...................................................................................................................... xxi

Chapter 1 ............................................................................................................................. 1

1 Introduction ...................................................................................................................... 1

1.1 DEM and experimental study on the effect of boundary condition on CPT calibration chamber tests .......................................................................................................................... 1

1.2 Comprehensive study on the effect of microparameters on CPT measurements ... 4

1.3 Instability of granular materials under simple shear failure mode: A DEM perspective .............................................................................................................................. 6

Chapter 2 ............................................................................................................................. 9

2 DEM and Experimental Study on the Effect of Boundary Condition on CPT Calibration Chamber Tests .................................................................................................................. 9

2.1 Introduction ................................................................................................................... 9

2.2 Experimental results used in this study ........................................................................ 14

2.3 Numerical DEM simulations ....................................................................................... 19

2.4 Results and discussions .............................................................................................. 29

  2.4.1 Model validation and preliminary results ............................................................... 29

  2.4.2 Effect of $D_{rc}$ and $\sigma'_{vc}$ .................................................................................. 32
2.4.3 Radial stress changes ........................................................................................................... 36
2.4.4 Force chain and displacement fields ................................................................................... 40
2.4.5 Correction for boundary effect ............................................................................................ 44
2.4.6 Comparison with other studies ............................................................................................ 45
2.5 Conclusion ............................................................................................................................... 47

Chapter 3 ....................................................................................................................................... 48

3 Comprehensive Study on the Effect of Microparameters on CPT Measurements ..... 48

3.1 Introduction ............................................................................................................................... 48

3.2 Numerical DEM simulations .................................................................................................... 52

3.2.1 Calibration of microparameters ........................................................................................... 52
3.2.2 DEM modeling methodology to simulate CPT ................................................................. 59
3.2.3 Fundamental aspects of the DEM granular assembly ......................................................... 67
3.2.4 Problem description and test series .................................................................................... 73

3.3 Results and discussions ........................................................................................................... 72

3.3.1 Effect of particle size ........................................................................................................... 72
3.3.2 Effect of relative density ...................................................................................................... 74
3.3.3 Effect of stress history ......................................................................................................... 86
3.3.4 Effect of effective modulus ($E^*$) ...................................................................................... 91
3.3.5 Effect of inter-particle friction coefficient ($\mu$) ............................................................... 100
3.3.6 Effect of particle shape (A.R and $\eta$) ............................................................................. 108
3.3.7 Effect of cone angle .......................................................................................................... 118
3.3.8 Compound effect of cone and sleeve friction coefficients .............................................. 124

3.4 Discussion on the effect of microparameters on soil behavior and CPT measurements .......................................................... 127

3.5 Conclusion ............................................................................................................................... 128

Chapter 4 ....................................................................................................................................... 130
List of Tables

Table 2-1: Different boundary conditions summarized by Salgado et al. (1998) ......................... 10

Table 2-2: Average and ultimate values of respectively $q_c$ and $f_s$ from CPT tests with BC1 and BC3 boundary conditions (Ganguly (2019)) .......................................................... 17

Table 2-3: Calibrated micromechanical parameters of the DEM simulation ......................... 22

Table 2-4: Summary of CPT DEM parameters used in this study ............................................ 26

Table 2-5: Total and relative (%) increases in $q_c$ from a BC1 to a BC5 boundary condition based on DEM simulations ........................................................................................................... 35

Table 2-6: Total and relative (%) increases in $q_c$ from a BC1 to a BC3 boundary condition from DEM simulations ........................................................................................................... 35

Table 3-1 DSS and Odometer simulation characteristics ................................................................. 55

Table 3-2: Calibrated micromechanical parameters of the DEM simulation ......................... 59

Table 3-3 Summary of the $V_s$ measurements ........................................................................ 70

Table 3-4: Test schedules and parameters used in this study ................................................. 65

Table 4-1: Calibrated micromechanical parameters used in this study ................................. 138

Table 4-2: Summary of the tests performed in this study .................................................... 147

Table 4-3 Summary of the coordination numbers at consolidation, instability and critical state for CV and DCSS simulations ................................................................. 166

Table 4-4 Summary of the DSS simulation results ................................................................. 133
List of Figures

Figure 1-1: Calculation procedure in a DEM cycle (O’Sullivan (2011)) ........................................... 3
Figure 1-2: Overview of the cone penetration test per ASTM D5778 .................................................. 5
Figure 1-3: Examples of DSS failure mode in shallow foundations and slopes................................. 7
Figure 2-1: Particle size distribution of Boler sand and the adopted DEM assemblies........ 15
Figure 2-2: Comparison of q_c and f_s between BC1 and BC3 conditions for specimens tested at an average \( \sigma'_{vc} = 403 \) kPa and \( D_{rc} = 67\% \) (Ganguly (2019)) .......................................................... 15
Figure 2-3: Comparison of q_c and f_s between BC1 and BC3 conditions for specimens tested at an average \( \sigma'_{vc} = 403 \) kPa and \( D_{rc} = 45\% \) (Ganguly (2019)) .......................................................... 16
Figure 2-4: Comparison of q_c and f_s between BC1 and BC3 conditions for specimens tested at an average \( \sigma'_{vc} = 102 \) kPa and \( D_{rc} = 26\% \) (Ganguly (2019)) .......................................................... 16
Figure 2-5: a) stress-strain, b) volumetric behavior and c) normal compression line (NCL) of calibrated DEM Direct Simple Shear and odometer tests and Experimental results performed by Mirbaha and Sadrekarimi (2017) .............................................................................. 21
Figure 2-6 Schematics of the DEM-based (a) DSS specimen, (b) Odometer specimen ........ 21
Figure 2-7 Variation of q_c for samples with different scaling factors ................................. 23
Figure 2-8: Illustration of different boundary conditions applied in the DEM simulations ... 24
Figure 2-9: Details of the cone and chamber cylinder used in this study ................................. 25
Figure 2-10: Variation of q_c for different sample heights ................................................................. 26
Figure 2-11: Comparisons of average q_c determined in the DEM simulations with those measured in the calibration chamber experiments (a) BC1, (b) BC3 ................................. 30
Figure 2-12: Profiles of $q_c$ at $\sigma'_vc = 400$ kPa for different $D_{rc}$ and a) BC1, b) BC3, and c) BC5 boundary conditions

Figure 2-13: Effect of boundary condition on the $q_c$ profiles at $D_{rc} = 65\%$ for a) $\sigma'_vc = 50$ kPa, b) $\sigma'_vc = 100$ kPa, c) $\sigma'_vc = 200$ kPa, d) $\sigma'_vc = 400$ kPa

Figure 2-14: Comparisons of $q_c$ for different boundary conditions and $D_{rc}$ for $\sigma'_vc$ of a) 400 kPa, b) 200 kPa, c) 100 kPa and d) 50 kPa

Figure 2-15: Effect of $\sigma'_vc$ on $q_c$ for different boundary conditions and $D_{rc}$

Figure 2-16: Variations of normalized radial stress with normalized penetration depth for samples consolidated to $\sigma'_vc$ of a) 50kPa, b) 100kPa, c) 200kPa and d) 400kPa at 25% relative density

Figure 2-17 Variations of normalized radial stress with normalized penetration depth for samples consolidated to $\sigma'_vc$ of a) 50kPa, b) 100kPa, c) 200kPa and d) 400kPa at 45% relative density

Figure 2-18 Variations of normalized radial stress with normalized penetration depth for samples consolidated to $\sigma'_vc$ of a) 50kPa, b) 100kPa, c) 200kPa and d) 400kPa at 65% relative density

Figure 2-19 Variations of normalized radial stress with normalized penetration depth for samples consolidated to $\sigma'_vc$ of a) 50kPa, b) 100kPa, c) 200kPa and d) 400kPa at 85% relative density

Figure 2-20: Strong force chain distribution and particle displacements at the end of penetration in loose assemblies ($D_{rc}=25\%$ and $\sigma'_vc=100$ kPa) with (a) BC1, (b) BC3 and BC5 boundary conditions

Figure 2-21: Strong force chain distribution and particle displacements at the end of penetration in very dense assemblies ($D_{rc}=85\%$ and $\sigma'_vc=100$ kPa) with (a) BC1, (b) BC3 and BC5 boundary conditions
Figure 2-22: Strong force chain distribution and particle displacements at the end of penetration in loose assemblies (D_{rc}=25\% and \sigma'_{vc}=400 \text{kPa}) with (a) BC1, (b) BC3 and BC5 boundary conditions................................................................. 43

Figure 2-23: Variations of CF with \sigma'_{vc}/P_a at different D_{rc} for (a) BC1 and (b) BC3 boundary conditions.................................................................................................................. 45

Figure 2-24: The correction coefficient based on various propositions and DEM for BC1 experiments with D_{rc}=45 and 65%.................................................................................................................. 46

Figure 3-1: PSD curve of the material used in this study for calibration ....................... 53

Figure 3-2: Schematics of a) DSS and b) odometer samples modeled for calibration using DEM.......................................................................................................................... 56

Figure 3-3: Funnel analysis test for assemblies with different \eta values and results; a) FRS, b) \eta=0.0, c) \eta=0.4, d) \eta=0.6 ................................................................. 57

Figure 3-4: a) stress-strain, b) volumetric behavior and c) coefficient of compressibility of calibrated DEM DSS and odometer tests and Experimental results................................. 58

Figure 3-5: Influence of particles finer than D_{10} in loose and very dense DEM assemblies reflected in terms of a) normalized q_c and b) normalized f_s ........................................... 60

Figure 3-6: variation of void ratios along the depth of the assemblies compared with the average void ratio measured from major RVE .............................................................................. 62

Figure 3-7: Schematics of the granular deposit and probe simulated using DEM ............ 63

Figure 3-8: Influence of penetration rate in loose DEM assemblies reflected in terms of a) normalized q_c and b) normalized f_s ............................................................................................... 65

Figure 3-9: Repeatability analysis for loose and very dense DEM assemblies reflected in terms of a) normalized q_c and b) normalized f_s .................................................................................. 66

Figure 3-10: Time history of the average particle velocity at different stress levels for the loose assembly caused by an impulse loading................................................................. 68
Figure 3-11: Variation of low strain shear wave velocities in terms of normalized vertical pressure for assemblies with different relative densities ................................................................. 69

Figure 3-12: Variations of horizontal stress, vertical stress and coefficient of pressure at rest (K0) for assemblies with a) $D_{rc}=25\%$, b) $D_{rc}=47\%$, c) $D_{rc}=67\%$ and d) $D_{rc}=85\%$ .................. 72

Figure 3-13: Soil behavior type chart of the modeled assemblies in different relative densities according to Robertson (2016) ( areas 1 to 9 represent Sensitive fine-grained, Organic, Clay, Silt mixtures, Sand mixtures, Sand, Gravelly sand to sand, Very stiff sand to clayey sand, and Very stiff fine-grained respectively) ........................................................................................................ 73

Figure 3-14: variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration of the assemblies with different $D_{c}/D_{50}$ ratios ................................................. 73

Figure 3-15 Variation of normalized shear wave velocity for assemblies with different particle sizes ($D_{c}/D_{50}$) ........................................................................................................ 73

Figure 3-16: variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) $q_{cN}$ in terms of normalized vertical pressure, d) $f_{sN}$ in terms of normalized vertical pressure, e) $q_{c1N}$ in terms of $f_{s1N}$ and f) SBT classification (Robertson (2016)) of the assemblies with different relative densities ........................................................................................................ 77

Figure 3-17: $D_{rc}$ and $q_{c1N}$ correlation obtained from DEM simulation for Fraser River Sand 78

Figure 3-18: Variations of a) $q_{cN}$ on normalized horizontal pressure and b) $f_{sN}$ on normalized horizontal pressure in different relative densities ................................................................. 78

Figure 3-19: Systematic grids of RVEs for porosity calculation and post-processing ........... 80

Figure 3-20: Void ratio distribution obtained in post processing for loose assembly in a) after consolidation b) after deep penetration ................................................................. 81

Figure 3-21: Void ratio distribution obtained in post processing for very dense assembly in a) after consolidation b) after deep penetration ................................................................. 81

Figure 3-22: Distribution of particle displacements at the end of penetration for (a) $D_{rc}=25\%$, (b) $D_{rc}=47\%$, (c) $D_{rc}=67\%$ and (d) $D_{rc}=85\%$ ........................................................................................................ 83
Figure 3-23: Distribution of particle velocity at the end of penetration for (a) $D_r=25\%$, (b) $D_r=47\%$, (c) $D_r=67\%$ and (d) $D_r=85\%$. ................................................................. 84

Figure 3-24: Strong contact force chain map distribution at the end of penetration for (a) $D_r=25\%$, (b) $D_r=47\%$, (c) $D_r=67\%$ and (d) $D_r=85\%$. ................................................................. 85

Figure 3-25: variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) normalized $q_c$ in terms of normalized vertical pressure, d) $q_{cN}$ in terms of OCR e) SBT classification and f) normalized shear wave velocity variation of the assemblies with different over-consolidation ratios (OCR) ................................................................. 88

Figure 3-26: Distribution of particle displacements in loose assemblies at the end of penetration with (a) OCR=1, (b) OCR=2, (c) OCR=4, (d) OCR=8 and (e) OCR=16........... 89

Figure 3-27: Strong contact force chain map distribution in loose assemblies at the end of penetration with (a) OCR=1, (b) OCR=2, (c) OCR=4, (d) OCR=8 and (e) OCR=16........... 90

Figure 3-28: variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) normalized $q_c$ in terms of normalized vertical pressure, d) $q_{c1N}$ in terms of $f_{s1N}$ and e) SBT classification of the assemblies with different $E^*$ ................................................................. 94

Figure 3-29: Shear wave velocity measurements for packings with different effective moduli ($E^*$) at loose and very dense relative densities ................................................................. 95

Figure 3-30: Distribution of particle displacements at the end of penetration in loose assemblies for (a) $E=50\text{MPa}$, (b) $E=100\text{MPa}$, (c) $E=150\text{MPa}$ and (d) $E=200\text{MPa}$............ 96

Figure 3-31: Distribution of particle displacements at the end of penetration in very dense assemblies for (a) $E=50\text{MPa}$, (b) $E=100\text{MPa}$, (c) $E=150\text{MPa}$ and (d) $E=200\text{MPa}$............ 97

Figure 3-32: Strong contact force chain map distribution at the end of penetration in loose assemblies for (a) $E=50\text{MPa}$, (b) $E=100\text{MPa}$, (c) $E=150\text{MPa}$ and (d) $E=200\text{MPa}$............ 98

Figure 3-33: Strong contact force chain map distribution at the end of penetration in very dense assemblies: (a) $E=50\text{MPa}$, (b) $E=100\text{MPa}$, (c) $E=150\text{MPa}$ and (d) $E=200\text{MPa}$............ 99
Figure 3-34: variation of a) $q_cN$ in terms of relative penetration, b) $f_sN$ in terms of relative penetration, c) normalized $q_c$ in terms of normalized vertical pressure, d) $q_{c1N}$ in terms of $f_{s1N}$ and e) SBT chart of the assemblies with different interparticle friction coefficient ($\mu$)...... 102

Figure 3-35: Shear wave velocity measurements for loose and very dense packings with different inter-particle friction ($\mu$)........................................................................................................ 103

Figure 3-36: Distribution of particle displacements at the end of penetration in loose assemblies with different inter-particle friction coefficients: (a) $\mu=0.05$, (b) $\mu=0.2$, (c) $\mu=0.4$, (d) $\mu=0.5$, (e) $\mu=0.6$ and (f) $\mu=0.7$ .................................................................................................................. 104

Figure 3-37: Distribution of particle displacements at the end of penetration in very dense assemblies with different inter-particle friction coefficients: (a) $\mu=0.05$, (b) $\mu=0.2$, (c) $\mu=0.4$, (d) $\mu=0.5$, (e) $\mu=0.6$ and (f) $\mu=0.7$ .................................................................................................................. 105

Figure 3-38: Strong contact force chain map distribution at the end of penetration in loose assemblies with different inter-particle friction coefficients: (a) $\mu=0.05$, (b) $\mu=0.2$, (c) $\mu=0.4$, (d) $\mu=0.5$, (e) $\mu=0.6$ and (f) $\mu=0.7$ .................................................................................................................. 106

Figure 3-39: Strong contact force chain map distribution at the end of penetration in very dense assemblies with different inter-particle friction coefficients: (a) $\mu=0.05$, (b) $\mu=0.2$, (c) $\mu=0.4$, (d) $\mu=0.5$, (e) $\mu=0.6$ and (f) $\mu=0.7$ .................................................................................................................. 107

Figure 3-40: a) Sample SEM image of Fraser river sand b) particle shapes simulated using DEM clump theory .................................................................................................................. 109

Figure 3-41: comparison of the variations of a) $q_cN$ on relative penetration, b) $f_sN$ on relative penetration, c) $q_cN$ in terms of normalized vertical pressure, d) $q_{c1N}$ in terms of $D_{rc}$ and e) SBT chart of the assemblies with different rolling resistance coefficient ($\eta$) and aspect ratios (A.R) .................................................................................................................. 113

Figure 3-42: Shear wave velocity measurements for the effects of rolling resistance coefficient ($\eta$) and particle shape (A.R) in loose and very dense assemblies....................... 113
Figure 3-43: Distribution of particle displacements at the end of penetration in loose assemblies with different rolling resistance coefficients: (a) $\eta=0$, (b) $\eta=0.2$, (c) $\eta=0.3$, (d) $\eta=0.4$ and (e) inhibited rolling

Figure 3-44: Distribution of particle displacements at the end of penetration in very dense assemblies with different rolling resistance coefficients: (a) $\eta=0$, (b) $\eta=0.2$, (c) $\eta=0.3$, (d) $\eta=0.4$ and (e) inhibited rolling

Figure 3-45: Strong contact force chain map distribution at the end of penetration in loose assemblies with different rolling resistance coefficients: (a) $\eta=0$, (b) $\eta=0.2$, (c) $\eta=0.3$, (d) $\eta=0.4$ and (e) inhibited rolling

Figure 3-46: Strong contact force chain map distribution at the end of penetration in very dense assemblies with different rolling resistance coefficients: (a) $\eta=0$, (b) $\eta=0.2$, (c) $\eta=0.3$, (d) $\eta=0.4$ and (e) inhibited rolling

Figure 3-47: Variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) normalized $q_c$ in terms of normalized vertical pressure, d) $q_{c1N}$ in terms of $f_{s1N}$ and e) SBT chart of the assemblies with different cone angles

Figure 3-48: Distribution of particle displacements at the end of penetration in loose assemblies with different cone angles: (a) $45^\circ$, (b) $60^\circ$, (c) $90^\circ$ and (d) $120^\circ$

Figure 3-49: Distribution of particle displacements at the end of penetration in very dense assemblies with different cone angles: (a) $45^\circ$, (b) $60^\circ$, (c) $90^\circ$ and (d) $120^\circ$

Figure 3-50: Strong contact force chain map distribution at the end of penetration in loose assemblies with different cone angles: (a) $45^\circ$, (b) $60^\circ$, (c) $90^\circ$ and (d) $120^\circ$

Figure 3-51: Strong contact force chain map distribution at the end of penetration in very dense assemblies with different cone angles: (a) $45^\circ$, (b) $60^\circ$, (c) $90^\circ$ and (d) $120^\circ$

Figure 3-52: Variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) $q_{cN}$ in terms of normalized vertical pressure, d) $q_{c1N}$ in terms of $f_{s1N}$ and e) SBT chart of the assemblies considering probe wear
Figure 3-53: SBT classification (Robertson (2016)) of the effect of all micro and macro parameters used in this study ................................................................. 128

Figure 4-1: PSD curve of Fraser river sand and the adopted assemblies ................................................. 136

Figure 4-2: Samples of a) Odometer test and b) Triaxial test simulated for calibration of micro-parameters ........................................................................................................... 137

Figure 4-3: Effect of lateral boundary friction on a) shear stress, b) volumetric strain.............. 140

Figure 4-4: Schematic of the (a) DEM assembly after consolidation, (b) DEM assembly end of shearing and (c) placement of RVEs in the specimen ......................................................... 141

Figure 4-5: Placements of embedded RVEs in a) xy plane and b) xz plane....................... 142

Figure 4-6: Void ratios measured from the RVEs after consolidation (e_c) in xz and yz planes for loose and dense assemblies .................................................................................. 143

Figure 4-7: Coefficients of earth pressure (k_0) obtained from the DEM simulations after consolidation .................................................................................................................. 144

Figure 4-8: Variations of I_{UF} throughout shearing in test with σ'_vc=100 kPa ...................... 144

Figure 4-9: Scaled-up specimens for DSS testing corresponding to a) 1053 particles, b) 5300 particles, c) 10380 particles, d) 21405 particles and e) 30000 particles (used in this study) 145

Figure 4-10: Variations of a) shear stress on shear strain and b) volumetric strain on shear strain for assemblies with different scaling factors at σ'_vc= 100 kPa ......................................... 146

Figure 4-11: Variations of a) Shear stress, b) volumetric strain and c) frictional angle of the DEM specimens in drained simple shear simulations ................................................. 149

Figure 4-12: a) mobilized friction angles obtained from DEM, α and β method, b) stress states on the Mohr circle for horizontal and vertical planes at the end of shearing.............. 150

Figure 4-13: stress states on the Mohr circle for horizontal and vertical planes at the end of shearing for a) Constant volume and b) Constant shear stress paths ............................... 151
Figure 4-14: Shear and normal stress distributions on the top plate at 20% shear strain for a) $\sigma'_{vc}=100\text{kPa}$, b) $\sigma'_{vc}=400\text{kPa}$ and c) $\sigma'_{vc}=700\text{kPa}$.

Figure 4-15: Shear and normal stress distributions on the top plate in undrained simulation with $\sigma'_{vc}=100\text{kPa}$: a) after consolidation b) instability c) critical state.

Figure 4-16: Variations of a) shear stress on shear strain, b) vertical effective stress on shear strain, c) pore water pressure on shear strain and d) stress path and critical state line for CV tests.

Figure 4-17: CSL obtained from DEM and experiments (Jones (2017)).

Figure 4-18: a) stress paths, b) volumetric strain, and c) accumulation of shear strain in DCSS simulations.

Figure 4-19: Evolution of strong contact force distribution a) after consolidation, b) at the onset of instability and c) at critical state in CV1 test.

Figure 4-20: Evolution of strong contact force distribution a) after consolidation, b) initiation of constant shear and c) onset of instability in DCSS1 test.

Figure 4-21: Particle displacements (a) after consolidation in CV1; (b) at the end of shearing in CV1 ($\sigma'_{vc}=100\text{kPa}$); (c) after consolidation in DCSS1; (d) at the end of shearing in DCSS1 ($\sigma'_{vc}=100\text{kPa}$); (e) after consolidation in CV8 and (f) at the end of shearing in CV8 ($\sigma'_{vc}=700\text{kPa}$).

Figure 4-22: Normalized cumulative particle rotation to the mean value in (a) onset of instability in DCSS1, (b) critical state in CV1 simulation.

Figure 4-23: Evolution of CN values in CV1 and DCSS1 tests.

Figure 4-24: Onset of instability presented for CV and DCSS tests at $\sigma'_{vc}=100, 200\text{kPa}$ in a) stress path, b) volumetric strain, c) accumulation of shear strain and d) second-order work variation.
Figure 4-25: Variations of a) yield friction angle on void ratio, b) yield friction angle on state parameter ($\psi_{cs}$) for CV and DCSS simulations.

136
List of Appendices

Appendix A-1: Profiles of $q_c$ at $\sigma'_{vc} = 200$ kPa for different $D_{rc}$ and a) BC1, b) BC3, and c) BC5 boundary conditions .......................................................... 153

Appendix B-2: Profiles of $q_c$ at $\sigma'_{vc} = 100$ kPa for different $D_{rc}$ and a) BC1, b) BC3, and c) BC5 boundary conditions ........................................................................ 154

Appendix C-3: Profiles of $q_c$ at $\sigma'_{vc} = 50$ kPa for different $D_{rc}$ and a) BC1, b) BC3, and c) BC5 boundary conditions ........................................................................ 155

Appendix D-3: Computation of the average stresses in the confines of the DSS assembly. 156

Appendix E-3: Radius Expansion Method (REM) used in the generation of some dense assemblies .................................................................................................................. 157
## Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Contact area</td>
</tr>
<tr>
<td>$A_c$</td>
<td>Cone surface area</td>
</tr>
<tr>
<td>AR</td>
<td>Aspect Ratio</td>
</tr>
<tr>
<td>$a_n$</td>
<td>Net area ratio</td>
</tr>
<tr>
<td>B</td>
<td>Skempton’s pore water pressure parameter</td>
</tr>
<tr>
<td>BC</td>
<td>Boundary Condition</td>
</tr>
<tr>
<td>BEM</td>
<td>Boundary Element Method</td>
</tr>
<tr>
<td>CA</td>
<td>Cone Angle</td>
</tr>
<tr>
<td>CC</td>
<td>Clay-like Contractive</td>
</tr>
<tr>
<td>CCS</td>
<td>Clay-like Contractive Sensitive</td>
</tr>
<tr>
<td>CD</td>
<td>Clay-like Dilative</td>
</tr>
<tr>
<td>CF</td>
<td>Correction Factor</td>
</tr>
<tr>
<td>CN</td>
<td>Coordination Number</td>
</tr>
<tr>
<td>CV</td>
<td>Constant Volume</td>
</tr>
<tr>
<td>CPT</td>
<td>Cone Penetration Test</td>
</tr>
<tr>
<td>CSL</td>
<td>Critical State Line</td>
</tr>
<tr>
<td>D</td>
<td>Dense</td>
</tr>
<tr>
<td>$D_c$</td>
<td>Diameter of chamber</td>
</tr>
<tr>
<td>$D_r$</td>
<td>Relative density</td>
</tr>
</tbody>
</table>
**D_{rc}**  Relative density after consolidation

**DCSS**  Drained Constant Shear Stress

**DEM**  Discrete Element Method

**DSS**  Direct Simple Shear

**DTT**  Drained Triaxial Test

**d_{c}**  Diameter of cone

**d_{max}**  Maximum particle size

**d_{10}**  Particle size with 10% passage in sieve analysis

**d_{s0}**  Average particle size

**E**  Effective modulus at contacts

**e_{c}**  Void ratio after consolidation

**e_{max}**  Maximum void ratio

**e_{min}**  Minimum void ratio

**F_{c}**  Total force acting on the frictional sleeve

**F^{(c)}**  Contact force vector

**\overrightarrow{F_{n}}**  Normal force vector

**\Delta \overrightarrow{F_{n}}**  Increment of normal force vector

**F_{r}**  Friction ratio

**\overrightarrow{F_{s}}**  Shear force vector

**\Delta \overrightarrow{F_{s}}**  Increment of shear force vector
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>FEM</strong></td>
<td>Finite Element Method</td>
</tr>
<tr>
<td><strong>FRS</strong></td>
<td>Fraser River Sand</td>
</tr>
<tr>
<td>$f_s$</td>
<td>Sleeve friction</td>
</tr>
<tr>
<td>$f_{sN}$</td>
<td>Dimensionless sleeve friction</td>
</tr>
<tr>
<td>$f_{s1N}$</td>
<td>Normalized dimensionless sleeve friction</td>
</tr>
<tr>
<td>$G$</td>
<td>Shear modulus</td>
</tr>
<tr>
<td>$G_s$</td>
<td>Specific gravity</td>
</tr>
<tr>
<td>$H$</td>
<td>Height of the specimen</td>
</tr>
<tr>
<td>IL</td>
<td>Instability Line</td>
</tr>
<tr>
<td>$I_{UF}$</td>
<td>Index of Unbalanced Forces</td>
</tr>
<tr>
<td>$k_n$</td>
<td>Normal stiffness</td>
</tr>
<tr>
<td>$k_{ratio}$</td>
<td>Normal to shear stiffness ratio</td>
</tr>
<tr>
<td>$k_s$</td>
<td>Shear stiffness</td>
</tr>
<tr>
<td>$k_r$</td>
<td>Rolling stiffness</td>
</tr>
<tr>
<td>L</td>
<td>Loose</td>
</tr>
<tr>
<td>$L^{(c)}$</td>
<td>Branch vector</td>
</tr>
<tr>
<td><strong>MCPT</strong></td>
<td>Miniature Cone Penetration Test</td>
</tr>
<tr>
<td>MD</td>
<td>Medium Dense</td>
</tr>
<tr>
<td>$\overline{Mr}$</td>
<td>Contact rolling moment</td>
</tr>
<tr>
<td>N</td>
<td>Scaling factor</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>NC</td>
<td>Normally Consolidated</td>
</tr>
<tr>
<td>NCL</td>
<td>Normal Compression Line</td>
</tr>
<tr>
<td>OC</td>
<td>Over Consolidated</td>
</tr>
<tr>
<td>Pa</td>
<td>Atmospheric pressure</td>
</tr>
<tr>
<td>PF</td>
<td>Particle Friction</td>
</tr>
<tr>
<td>PFC</td>
<td>Particle Flow Code</td>
</tr>
<tr>
<td>PSD</td>
<td>Particle Size Distribution</td>
</tr>
<tr>
<td>Qc</td>
<td>Total force acting on the cone</td>
</tr>
<tr>
<td>Qtm</td>
<td>Normalized total cone tip resistance</td>
</tr>
<tr>
<td>qc</td>
<td>Cone tip resistance</td>
</tr>
<tr>
<td>qcb</td>
<td>Measured cone tip resistance</td>
</tr>
<tr>
<td>qce</td>
<td>Corrected cone tip resistance</td>
</tr>
<tr>
<td>qcn</td>
<td>Dimensionless cone tip resistance</td>
</tr>
<tr>
<td>qcin</td>
<td>Normalized dimensionless cone tip resistance</td>
</tr>
<tr>
<td>Ra</td>
<td>Particle radius</td>
</tr>
<tr>
<td>RR</td>
<td>Rolling Resistance</td>
</tr>
<tr>
<td>RVE</td>
<td>Representative Volume Element</td>
</tr>
<tr>
<td>SBT</td>
<td>Soil Behavior Type</td>
</tr>
<tr>
<td>SC</td>
<td>Sand-like contractive</td>
</tr>
<tr>
<td>SD</td>
<td>Sand-like dilative</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>--------</td>
<td>----------------------------------</td>
</tr>
<tr>
<td>$S_u$</td>
<td>Undrained shear strength</td>
</tr>
<tr>
<td>TC</td>
<td>Transitional Contractive</td>
</tr>
<tr>
<td>TD</td>
<td>Transitional Dilative</td>
</tr>
<tr>
<td>$\Delta \bar{U}_n$</td>
<td>Increment of relative normal displacement</td>
</tr>
<tr>
<td>$\Delta \bar{U}_s$</td>
<td>Increment of relative shear displacement</td>
</tr>
<tr>
<td>$\Delta \bar{\omega}_r$</td>
<td>Increment of relative rotation</td>
</tr>
<tr>
<td>$u_w$</td>
<td>Pore water pressure</td>
</tr>
<tr>
<td>$V$</td>
<td>Vessel volume</td>
</tr>
<tr>
<td>VCC</td>
<td>Virtual Calibration Chamber</td>
</tr>
<tr>
<td>VD</td>
<td>Very Dense</td>
</tr>
<tr>
<td>$V_s$</td>
<td>Shear wave velocity</td>
</tr>
<tr>
<td>W</td>
<td>Second-order work</td>
</tr>
<tr>
<td>$\alpha_d$</td>
<td>Non-local damping ratio</td>
</tr>
<tr>
<td>$\dot{\gamma}$</td>
<td>Strain rate</td>
</tr>
<tr>
<td>$\sigma'_h$</td>
<td>Effective horizontal stress</td>
</tr>
<tr>
<td>$\sigma'_v$</td>
<td>Effective vertical stress</td>
</tr>
<tr>
<td>$\sigma'_{vc}$</td>
<td>Effective vertical stress after consolidation</td>
</tr>
<tr>
<td>$\sigma'_{vcs}$</td>
<td>Effective vertical stress at critical state</td>
</tr>
<tr>
<td>$\sigma'_1$</td>
<td>Maximum principal stress</td>
</tr>
<tr>
<td>$\sigma'_2$</td>
<td>Intermediate principal stress</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td>$\sigma'_{3}$</td>
<td>Minimum principal stress</td>
</tr>
<tr>
<td>$\overline{\sigma_{ij}}$</td>
<td>Average stress tensor</td>
</tr>
<tr>
<td>$\dot{\sigma}'$</td>
<td>Tensor of second-order effective stress</td>
</tr>
<tr>
<td>$\varepsilon_a$</td>
<td>Axial strain</td>
</tr>
<tr>
<td>$\varepsilon_h$</td>
<td>Horizontal strain</td>
</tr>
<tr>
<td>$\varepsilon_r$</td>
<td>Radial strain</td>
</tr>
<tr>
<td>$\varepsilon_v$</td>
<td>Vertical strain</td>
</tr>
<tr>
<td>$\varepsilon_{vol}$</td>
<td>Volumetric strain</td>
</tr>
<tr>
<td>$\dot{\varepsilon}'$</td>
<td>Tensor of second-order total strain</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Shear stress</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Inter-particle rolling resistance coefficient</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Inter-particle friction coefficient</td>
</tr>
<tr>
<td>$\phi'_{cs}$</td>
<td>Friction angle at critical state</td>
</tr>
<tr>
<td>$\phi'_{mob}$</td>
<td>Mobilized friction angle</td>
</tr>
<tr>
<td>$\phi'_{yield}$</td>
<td>Yield friction angle</td>
</tr>
<tr>
<td>$\chi$</td>
<td>Dimensionless rolling resistance coefficient</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Dilation angle</td>
</tr>
<tr>
<td>$\psi_{es}$</td>
<td>State parameter</td>
</tr>
<tr>
<td>$\Delta h$</td>
<td>Relative depth</td>
</tr>
<tr>
<td>$\Delta \sigma'_{h}$</td>
<td>Increment of effective horizontal stress</td>
</tr>
</tbody>
</table>
Δ\sigma'_v \quad \text{Increment of effective vertical stress}

Δ\epsilon_h \quad \text{Increment of horizontal strain}

Δ\epsilon_v \quad \text{Increment of vertical strain}
Chapter 1

1 Introduction

This chapter presents a review of the literature on Cone Penetration Test and DSS tests for comparison and validation purposes.

1.1 DEM and experimental study on the effect of boundary condition on CPT calibration chamber tests

Geotechnical design projects require accurate site characterization, soil stratigraphy, and strength parameters. In-situ assessment of these parameters is of utmost importance specifically in cohesionless soils from which taking undisturbed samples seem an onerous task. Therefore, many attempts have been made to correlate the parameters obtained in in-situ tests and design parameters of soils.

Extensive research has been conducted trying to correlate between these parameters and mechanical properties of soil such as friction angle, relative density and unit weight (e.g., Schmertmann (1978a), Jamilokowski et al. (2003)). However, conducting CPT for research purposes is neither economically feasible, nor possible in remote areas. Therefore, numerous attempts have been made to investigate the cone penetration in laboratory-scale tests namely calibration chambers. Calibration chambers often contain large quantities of soil and suffer from inhomogeneity in the soil medium. Miniature Cone Penetration Tests (MCPT), an alternative to the problematic size of calibration chambers, also present notable boundary and scale effects. For this reason, five different boundary conditions namely BCi (i varies between 1 to 5) are expected to apply on a soil assembly. The details of the stresses and strains applied in each boundary condition is described in detail in chapter 2.

BC1 and BC3 boundary conditions are frequently investigated among practitioners. Parkin and Lunne (1982) reported that in a chamber, the actual values of cone resistance are between these two bands. Constant stress boundary condition (BC1) is the lower band since the stresses in the centerline of the chamber are lower than that of the field.
Contrarily, constant strain boundary condition (BC3) imposed higher stress values at the centerline of the chamber than those observed in the field, leading to higher cone resistance values. On the same basis, Parkin and Lunne (1982), Been et al. (1987), Mayne and Kulhawy (1991), Schnaid and Houlsby (1991), Wesley (2002a), Sadrekarimi (2016) studied and developed calibration chambers and proposed correction factors to obtain the free-field cone resistance (BC5). The application of free-field boundary condition (BC5) is quite difficult in a laboratory setting. Furthermore, the variations of normalized radial stress have not been investigated in the centerline of calibration chambers due to difficulties in instrumentation set-up.

Discrete Element Method (DEM) developed by Cundall and Strack (1979) seems a promising solution for the aforementioned problems observed in calibration chambers. In DEM, soil grains are modeled as discrete elements interacting at contacts with micromechanical constitutive models. These models include springs, dashpots, and sliders to represent the various degrees of freedom locally. First, the Interparticle forces are calculated using the micro parameters and the force exerted on the system. Using Newton’s second law of motion, the acceleration of the assembly, and by considering an infinitesimal timestep, the velocity and displacement of the particles are calculated. This cycle continues until the assembly reaches equilibrium (Figure 1-1).

The first DEM-based virtual calibration chamber (VCC) was developed by Arroyo et al. (2011). The particle assembly was calibrated to capture the behavior of Ticino sand. Cone penetration tests were simulated by a cone with $D_c/d_c = 16.8$ on DEM models with particles scaled by a factor of 50. BC1 and BC3 boundary conditions were chosen as the baseline simulations in this study. A significant increase was observed in cone tip resistance values when the radial boundary condition altered from constant stress (BC1) to constant strain (BC3) condition. In the same vein, Falagush et al. (2015b) simulated a miniature calibration chamber using DEM. The particles were generated using the radius expansion method. The stress in the radial direction was controlled through a servo-controlled mechanism. It was observed that $q_c$ values are highly sensitive to the particle crushing.
Utilizing the asymmetry of the calibration chambers, Lin and Wu (2012) developed a miniature calibration chamber by only simulating a 30° section to investigate the effect of various cone sizes on CPT measurements. The particles were settled under gravity and then compressed using servo-mechanism. It was observed that reducing the cone size increased the cone resistance and sleeve friction. The effect of vertical stress and relative density coupled with volume-based calculations embedded in PFC will subsequently be discussed in chapter 2 to investigate the boundary conditions comprehensively.
1.2 Comprehensive study on the effect of microparameters on CPT measurements

The Cone Penetration Test (CPT) is an in-situ testing method that is widely used to characterize the subsurface soil and obtain its geotechnical parameters. It has become one of the most popular testing methods due to its repeatability, rapidity and accuracy. Figure 1-2 presents the conventional CPT standardized by ASTM D 5778. The test consists of continuous penetration of series of rods into the ground at a constant rate of 20 mm/s. The rod is composed of a cone with 60° apex angle and 10 cm² surface area at the base level and a friction sleeve with a surface area of 150 cm².

In CPT, the soil properties are obtained indirectly from the soil response to the penetration. The provided responses are cone resistance $q_c$ (total force acting on the cone divided by its surface area, $Q_c/A_c$) and sleeve friction $f_s$ (total force acting on the friction sleeve divided by its surface area, $F_c/A_s$). Recently, pore pressure piezometers have been implemented in the cone to measure this parameter as well for soil stratigraphy purposes. The capability and accuracy of CPT in soil characterization and obtaining geotechnical parameters has made this test a point of interest for engineers and practitioners. However, it is economically and physically impossible to perform in-situ CPT tests for research purposes. For this reason, many researchers (Vesic (1972), Janbu and Senneset (1974), Durgunoglu and Mitchell (1975), Salgado et al. (1997), Yu (2000)) and numerical approaches (Baligh (1985), Teh and Houlsby (1991), Sagaseta et al. (1997), Abu-Farsakh et al. (1998), Lu et al. (2004), Ahmadi and Robertson (2005), Moug et al. (2016), Gupta et al. (2016)) have utilized numerical and analytical approaches to investigate the penetration problems in a soil medium.

The prevalent assumptions in continuum mechanics may contradict with the distinct nature of soils, specifically in large deformation problems such as CPT. Therefore, Discrete Element Method (DEM) with a distinct nature can overcome these challenges, without requiring complex constitutive models or adaptive remeshing techniques. DEM is a promising tool to investigate the effect of micro and macro parameters on CPT measurements.
Few studies have focused on CPT in a 3D-soil medium using DEM. This is due to the high computational effort resulted with high number of spheres. Using a coupled DEM-BEM platform, An-Bin Huang and Ma (1994) developed a plane-strain model to simulate CPT in a granular medium. Their results show that both the penetration mechanism and soil dilatancy in a granular material are affected by its loading history. Jiang et al. (2006b) used a 2D-DEM model to investigate the soil-cone interface friction. It was observed that the cone resistance increases with increasing depth and tip-soil friction coefficient. High gradients of particle rotation, particle displacements and velocity fields are generated around the cone tip throughout the penetration. On the same basis, they investigated the inclined penetration mechanism in granular medium. Several penetration tests were carried out with different inclination angles with respect to the ground surface. An increase was observed in the normalized cone tip resistance with inclination angle.

Khosravi et al. (2019) studied the effect of micro and macro parameters on CPT measurements and classification using a DEM-based calibration chamber. While giving some valuable insight on the effect of particle friction and rolling resistance, very limited
range of parameters were investigated in this study. The complete study on the effect of micro parameters of a novel constitutive model that accounts for particle shape (Rolling resistance model) on CPT measurements and soil classification behavior will subsequently be discussed in chapter 3.

1.3 Instability of granular materials under simple shear failure mode: A DEM perspective

Direct Simple Shear (DSS) tests is used nowadays to define the strength parameters of soil in static or cyclic loadings. The plane-strain boundary condition, \( k_0 \) consolidation and the rotation of principal stresses applied in this device has led to its popularity among practitioners. The first DSS device was made by the Royal Swedish Geotechnical Institute in 1936 to capture the “True” simple shear conditions. The mentioned device was developed by Kjellman (1951) and is famous by the name “NGI” among practitioners. In NGI device, the cylindrical model is confined with a set of strings and shear is applied by the horizontal boundaries. In another device developed by Roscoe (1953), the shear is applied to the cubical specimen by the rotation of rigid lateral walls. The DSS stacked-ring (Ishihara and Yamazaki (1980)) is the most common device used by the practitioners in which the specimen is confined with a set of steel rings. The shear can be applied by the movement of the horizontal plate in two perpendicular directions.

In this device, the state of stress remains unknown throughout the shearing since the distribution of lateral stresses is not measured. The instrumentation of the device has some challenges due to the limited size of the specimen. Moreover, the stress-strain distribution along the boundaries is non-uniform since the smooth radial boundary condition impedes the complementary coupled shearing stress components from generation. Consecutive limitations of the device and the inaccurate assumptions used in continuum mechanics makes DEM an appropriate tool in the investigation of simple shearing failure mode.

The first attempt in DEM simulation of simple shear test was carried out by Matsuoka et al. (1988). Using plane-strain simulation of Cambridge type DSS on Aluminum bars, they observed that the principal stresses rotate as much as 35% after the peak strength
(about 5%). Peña et al. (2007) used imaging technics to simulate particle shapes with 4 and 10 element clumps that mimic the sands in Japan. Simulating constant volume and constant stress simple shearing, they captured the static liquefaction perfectly. However, the void ratios obtained in this study were not accurately modeled with clumps, suggesting that more complex constitutive models are required.

**Figure 1-3: Examples of DSS failure mode in shallow foundations and slopes**

Zhang and Evans (2018) studied the effect of different boundary conditions in both cyclic DSS and Triaxial tests. Rigid and periodic boundaries were compared in simulation of liquefaction behavior in loose granular assemblies. In a periodic system, materials behave as the cell is infinite in each facet, allowing particles to exit from one facet and enter from the adjacent parallel facet. On the other hand, the displacement of particles in contact with the rigid boundaries is controlled by a set of springs and dashpots, primarily stiffer
than that of inter-particle values. They observed that specimens with stiff boundaries have more extensive changes in contact anisotropy during shearing. This is due to the restrain of particle movements along the stiff boundaries.

Despite the discrepancies, DSS is widely applied to evaluate the liquefaction potential of soils. In a granular material, instability occurs when the medium is unable to sustain the applied load. Liquefaction is a form of instability that occurs in loose granular materials due to pore water pressure generation that is triggered by the undrained shear loading prior to failure (Sadrekarimi (2020)). Another form of instability that occurs in fully drained condition is triggered by the reduction in mean principal effective stress associated with an increase in pore pressure, in constant shear stress. (Skopek et al. (1994), Chu et al. (2003), Daouadji et al. (2010), Dong et al. (2016)). The onset of instability in such drained failures is very critical as no peak stress is observed in the stress path applied. The conditions leading to drained and undrained instability, various criteria in determining the onset of instability, and the methods in defining the strength parameters will subsequently be discussed in chapter 4.
Chapter 2

2 DEM and Experimental Study on the Effect of Boundary Condition on CPT Calibration Chamber Tests

Laboratory controlled CPTs with miniature cones and reduced-scale calibration chamber devices are often challenged by boundary effects on measured penetration resistances. For this purpose, a series of Discrete Element Simulations (DEM) are performed and compared with experimental calibration chamber tests to investigate the influence of boundary conditions on cone tip ($q_c$) and sleeve frictional ($f_s$) resistances. Based on these findings, specific correction factors are proposed to better estimate the free field penetration resistances.

2.1 Introduction

Cone Penetration Tests (CPT) are widely used as an investigation tool for in-situ geotechnical characterization. It is highly preferred because of its simplicity, excellent repeatability and capability of providing continuous data along with the depth of penetration. As CPT does not directly measure any soil properties, widespread research has been conducted to develop empirical correlations of CPT measurements with engineering properties such as relative density, unit weight and modulus using laboratory calibration chamber experiments (Sadrekarimi 2016). Carrying out conventional laboratory-based calibration chamber tests with a standard cone (diameter of 35.7 mm) requires a large diameter chamber (typically 1.2 m). Such an experiment can be difficult to carry out as preparing the soil sample is time-consuming and the control over sample uniformity and external stresses are often challenged due to its large dimensions. Due to these disadvantages, researchers have focused on building reduced-scale calibration chambers and miniature cone penetrometers (Abedin 1995; Huang and Hsu 2005; Kumar and Raju 2009; Pournaghiazar et al. 2011). Although using a smaller calibration can be more convenient, it leads to uncertainties about the influence of the specimen boundary on the measured penetration resistances. Past literature has shown that the diameters of the cone penetrometer and the soil sample are both conducive to the influence of lateral boundaries in a calibration chamber. In an in-situ Cone Penetration test, the soil medium
has no boundaries as the horizontal and vertical boundaries are at nearly infinite distances from the cone. CPT resistances measured in a calibration chamber test can be different from in-situ measurements because of the limited size of a calibration chamber and the imposed boundary effect on cone tip ($q_c$) and sleeve ($f_s$) resistances. Hence, the chamber size effect needs to be considered in predicting field performance or verifying and establishing new correlations between cone resistance and soil properties from calibration chamber test results. The effect of chamber size and boundary conditions is examined in this study through both numerical discrete element analyses and experimental CPT calibration chamber tests. Depending on whether stresses (horizontal: $\sigma_h'$; vertical: $\sigma_v'$) or strains (horizontal: $\varepsilon_h$; vertical: $\varepsilon_v$) on the sample boundaries are kept constant, a cylindrical sample can be subjected to four different boundary conditions as summarized by Salgado et al. (1998) in Table 2-1.

**Table 2-1: Different boundary conditions summarized by Salgado et al. (1998)**

<table>
<thead>
<tr>
<th>Boundary condition</th>
<th>Lateral condition</th>
<th>Top/bottom condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>BC1</td>
<td>$\Delta \sigma_h' = 0$</td>
<td>$\Delta \sigma_v' = 0$</td>
</tr>
<tr>
<td>BC2</td>
<td>$\Delta \varepsilon_h = 0$</td>
<td>$\Delta \varepsilon_v = 0$</td>
</tr>
<tr>
<td>BC3</td>
<td>$\Delta \varepsilon_h = 0$</td>
<td>$\Delta \sigma_v' = 0$</td>
</tr>
<tr>
<td>BC4</td>
<td>$\Delta \sigma_h' = 0$</td>
<td>$\Delta \varepsilon_v = 0$</td>
</tr>
</tbody>
</table>

Several researchers have studied the influence of boundary conditions on $q_c$ and $f_s$ measured in a calibration chamber test. The effect of sample boundaries is generally assessed based on the ratio of the calibration chamber diameter ($D_c$), to the cone diameter ($d_c$). This corresponds to $D_c/d_c = 25$ for the CPT calibration chamber experiments carried out in this study, with $d_c = 6$ mm and $D_c = 150$ mm. In CPT calibration chamber tests on Hokksund sand, Parkin and Lunne (1982) observed little effect of chamber size for loose samples as $D_c/d_c$ increased from 22 to 48. However, for dense specimens, they showed that $D_c/d_c > 50$ was required to minimize boundary effects. Baldi et al. (1981) performed cone penetration tests in a calibration chamber using dry normally consolidated (NC) and
over consolidated (OC) Ticino sand prepared to sample height and diameter of 1.5 m and 1.2 m, respectively. A conventional Fugro-type cone penetrometer having a diameter of 35 mm was used which resulted in $D_c/d_c$ ratio of 32. The authors tested samples having relative densities ranging from 35% to 96% and observed that higher $q_c$ values in BC3 boundary condition compared to BC1, which was more pronounced in dense specimens. Conclusively, they associated the increased $q_c$ to the higher radial stress around the cone during penetration with rigid boundaries (BC3) that increased the load response at the cone tip. Bolton and Gui (1993) performed CPT tests using a 10 mm cone penetrometer in centrifuge models of Fontainbleau sand with diameters of 210, 420 and 850 mm at a relative density of 76% and realized lateral boundary effects at a $D_c/d_c$ ratio of 21. However, no boundary effects were observed even at a relative density of 90% when $D_c/d_c$ ranged from 42 to 85. Bolton et al. (1999) used uniformly graded Fontainbleau sand sample diameters of 850 mm and 210 mm for a 10 mm diameter cone probe, and sample diameters of 530 mm and 100 mm for cone diameters of 12 mm and 11.3 mm, which provided a $D_c/d_c$ ratio range of 8.85 to 85. The authors performed the tests at sample relative densities of 80-85% and reported significant boundary effect on penetration resistances at $D_c/d_c$ of 8.85.

On the other hand, a negligible boundary effect was found by Ahmadi (2000) in numerical finite-difference simulations of CPT in Ticino sand at $D_{rc} = 50\%$. Similarly, Esquivel and Silva (2000) also found little boundary effects from calibration chamber tests on Nevada #100 sand prepared to a sample diameter of 572 mm and using two different cone penetrometers with $d_c = 12.7$ mm and 19.5 mm producing $D_c/d_c$ ratios of 30 and 45, respectively. The cones were pushed at different positions of the sample top surface, yet negligible boundary effects were reported by the authors. de Jong et al. (2007) performed laboratory tests on 0.028 m$^3$ of overconsolidated blocks of Connecticut Valley varved clay samples to enable assessment of deformation fields induced by a piezocone. The samples were penetrated with a specially designed cone penetrometer with a diameter of 12.7 mm extending for a certain shaft length after which it broadened at an angle of 15 degrees to a diameter of 44.5 mm. After carefully observing any lateral deformation and dissecting the samples to study the inner deformation pattern, the
authors reported that a \( \frac{D_c}{d_c} \) ratio of 24 was adequate to eliminate any lateral boundary effect.

Huang and Hsu (2005) performed a field simulator calibration chamber test with a specimen height and diameter of 1600 mm and 790 mm, respectively. A constant uniform stress was applied to the top and bottom boundaries of the sample while a deformable lateral boundary was imposed by a stack of 20 rubber rings around the specimen. The cone penetration made the specimen boundary to expand and the rubber rings to stretch as the cone tip traveled through the specimen. This deformable boundary condition imposed by the rubber rings was neither a constant stress nor a zero-strain condition. It was called a simulated field boundary condition (BC5). These tests were done on a batch of quartz sand from Da Nang, Vietnam using two cones with diameters of 17.8 mm and 35.7 mm, providing \( \frac{D_c}{d_c} = 44 \) and 22, respectively.

Conducting in-situ CPT for research purposes is neither economically feasible, nor possible in remote areas or the field. For this reason, researchers have used analytical and numerical approaches to investigate the mechanism of cone penetration such as the bearing capacity (Terzaghi (1943)), cavity expansion (Yu (2000), strain path (Baligh (1985), Sagaseta et al. (1997)) finite element (Abu-Farsakh et al. (1998), Gupta et al. (2016)) methods. Most of these methods are only applicable to loose to medium-dense sands as they don’t account for the dilatant behavior of dense sands. A series of numerical simulations and CPT calibration chamber tests were conducted by Goodarzi et al. (2018). In the experimental setting, a miniature cone with a diameter of 12 mm was pushed into Cuxhaven sand samples with relative densities \( (D_{rc}) \) of 75% and 95%. The 300 mm wide sample was subjected to different boundary conditions, resulting in the highest \( q_c \) in BC3, following by BC5 and then BC1 conditions for the same \( D_{rc} \) and stress conditions. These observations were also confirmed by a series of numerical penetration analyses in an infinite soil mass to evaluate the implemented constant stiffness boundary condition in the chamber Goodarzi et al. (2018).
The effect of different boundary conditions on \( q_c \) and \( f_s \) are studied in this study through a series of reduced-scale calibration chamber tests and numerical discrete element models (DEM). These are described in the following paragraphs.

The large-deformation nature of CPT requires the use of complex constitutive models (Butlanska et al. (2014b)) in continuum-based numerical analysis. In contrast, the inherent distinct nature of DEM can capture the particulate interactions occurring in granular media at micro and macro levels using Newton’s Laws of Motion. DEM was first introduced by Cundall and Strack (1979) as a novel technique for modeling in rock mechanics and since has been widely used in different aspects of modeling granular media. Several investigators (Huang et al. (1993), Nova (2005), Jiang et al. (2006a), Arroyo et al. (2011), Lin and Wu (2012), Butlanska et al. (2014b), Falagush et al. (2015a), Ciantia et al. (2016), Khosravi et al. (2019), Peters et al. (2019)) have used DEM to simulate a CPT. Huang et al. (1993) present the first application of DEM in simulating CPT in sand. They show that the cone penetration mechanism and dilatancy are affected by the loading history. Jiang et al. (2006b) used a two-dimensional -DEM model with the focus on soil-cone interface friction. It was found that \( q_c \) increased with increasing depth and cone interface friction. At the micro-level, high gradients of particle rotation, particle displacements and velocity fields were observed around the cone tip. All details considered, a plane strain simulation of CPT is incapable of representing the actual behavior of granular media due to differences in contact geometry and porosity calculations (Falagush et al. (2015a)).

Butlanska et al. (2014b) developed a virtual calibration chamber (VCC) using a 3D-DEM approach to perform cone penetration tests on a discrete analogue of Ticino sand. Cone penetration tests were simulated by a cone with \( D_c/d_c = 16.8 \) on DEM models with particles scaled by a factor of 50. BC1 and BC3 were chosen as a series of boundary conditions applied to the specimen. A change in the radial boundary condition from BC1 to BC3 in this study resulted in a significant increase in cone resistance. A miniature cone penetration test (MCPT) was modelled by Lin and Wu (2012) using 3D-DEM to investigate the effect of cone diameter and geometry on cone resistance. It was observed that reducing the cone size increased the cone resistance and sleeve friction. Based on 3D
discrete element simulations of CPT with particle gradation of Ticino sand, Butlanska et al. (2010) showed that boundary effect diminished as $D_c/d_c > 22$ for $D_{rc} = 75\%$. The results of simulations with a smaller cone diameter exhibited larger oscillations due to the smaller cone diameter to particle size ratio ($d_c/D_{50}$).

Despite some discrepancies, most studies generally indicate that penetration tests performed at small $D_c/d_c$ ratios often have a lower penetration resistance than those at greater $D_c/d_c$ ratios, and the effect of boundary condition on penetration resistance is generally more substantial with increasing relative density. Therefore, within the confines of this paper, it is attempted to investigate the influence of boundary conditions on clean sand specimens using both experimental and numerical (DEM) approaches. The goal is to determine the specimen size that would minimize sample boundary effects or factors to correct cone resistance with respect to boundary conditions in smaller diameter samples.

### 2.2 Experimental results used in this study

For the experimental results of this study, a CPT calibration chamber was originally developed by Damavandi-Monfared and Sadrekarimi (2015) and later upgraded by Jones (2017) to allow anisotropic consolidation and the measurement of shear wave velocity. The calibration chamber can fit a specimen with a height of 190 mm and a diameter of 150 mm. A 6 mm diameter miniature cone penetrometer probe with an apex angle and the net area ratio ($a_n$) of 60 degrees and 0.75, respectively is used in this study, which provides a $D_c/d_c = 25$. Reconstituted specimens of a local silica sand designated as “Boler Sand” were prepared and tested in this experimental program (Ganguly (2019)). A special testing program was designed and conducted in this study to examine the effect of sample boundaries cone penetration and sleeve frictional resistances between BC1 and BC3 boundary conditions. Figure 2-2 to Figure 2-4 compare $q_c$ and $f_s$ profiles between BC1 and BC3 boundary conditions for different $D_{rc}$ (Ganguly (2019)). According to these figures, the largest difference between BC1 and BC3 cone penetration resistances is observed in the dense specimens ($D_{rc} = 65\%$) which reduces with $D_{rc}$ and nearly diminishes at $D_{rc} = 25\%$. This is consistent with prior research (Houlsby and Hitchman 1988; Mayne and Kulhawy 1991; Schnaid and Houlsby 1991; Salgado et al. 1998) which show that the influence of boundary condition is higher in dense specimens.
Figure 2-1: Particle size distribution of Boler sand and the adopted DEM assemblies

![Particle size distribution graph]

D_{max} = 0.845 mm
D_{min} = 0.525 mm

Figure 2-2: Comparison of $q_c$ and $f_s$ between BC1 and BC3 conditions for specimens tested at an average $\sigma'_vc = 403$ kPa and $D_{rc} = 67\%$ (Ganguly (2019))

![Comparison graph]
Figure 2-3: Comparison of $q_c$ and $f_s$ between BC1 and BC3 conditions for specimens tested at an average $\sigma'_{vc} = 403$ kPa and $D_{rc} = 45\%$ (Ganguly (2019))

Figure 2-4: Comparison of $q_c$ and $f_s$ between BC1 and BC3 conditions for specimens tested at an average $\sigma'_{vc} = 102$ kPa and $D_{rc} = 26\%$ (Ganguly (2019))
As illustrated in Figure 2-2 to Figure 2-4, $q_c$ continues to increase with depth until a certain critical depth (at about 25-30 mm), beyond which $q_c$ seems to plateau whereas $f_s$ continues to decrease as the circumferential area of the sleeve increases with penetration depth. The average values of $q_c$ and $f_s$ after reaching their respective plateaus from all CPT experiments are summarized in Table 2-2 (Ganguly (2019)).

Table 2-2: Average and ultimate values of respectively $q_c$ and $f_s$ from CPT tests with BC1 and BC3 boundary conditions (Ganguly (2019))

<table>
<thead>
<tr>
<th>BC</th>
<th>$D_{rc}$ (%)</th>
<th>$\sigma'_{ve}$ (kPa)</th>
<th>$q_c$ (MPa)</th>
<th>$f_s$ (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BC1</td>
<td>27.2</td>
<td>99</td>
<td>6.8</td>
<td>73.7</td>
</tr>
<tr>
<td>BC3</td>
<td>24.7</td>
<td>105</td>
<td>6.9</td>
<td>76.8</td>
</tr>
<tr>
<td>BC1</td>
<td>47.8</td>
<td>406</td>
<td>19.1</td>
<td>185.9</td>
</tr>
<tr>
<td>BC3</td>
<td>43.7</td>
<td>400</td>
<td>17.8</td>
<td>173.2</td>
</tr>
<tr>
<td>BC3</td>
<td>44.5</td>
<td>402</td>
<td>18.4</td>
<td>172.9</td>
</tr>
<tr>
<td>BC1</td>
<td>67.2</td>
<td>402</td>
<td>23.4</td>
<td>231.4</td>
</tr>
<tr>
<td>BC1</td>
<td>65.7</td>
<td>405</td>
<td>22.7</td>
<td>222.2</td>
</tr>
<tr>
<td>BC3</td>
<td>68.2</td>
<td>400</td>
<td>25.8</td>
<td>283.4</td>
</tr>
<tr>
<td>BC3</td>
<td>67.4</td>
<td>405</td>
<td>26.1</td>
<td>278.7</td>
</tr>
</tbody>
</table>

As shown in Figures 2-2 through 2-4 as well as in Table 2-2, there is little effect of boundary condition in loose ($D_{rc} = 25\%$) and medium-dense ($D_{rc} = 45\%$) samples. However, for the dense samples ($D_{rc} = 65\%$) the $q_c$ shows an increase of approximately 3 MPa in BC3 condition, corresponding to an increase of about 12.7%,
compared to those measured in samples subjected to BC1 condition. Similarly, $f_s$ has increased by an average of 54 kPa from BC1 to BC3 condition, which corresponds to an increase of 24% in dense samples. The boundary condition has a more pronounced effect on $f_s$ (than $q_c$) as sand dilatancy is mobilized on a larger surface area than that of the cone tip. In summary, the experimental results indicate a noticeable increase in $q_c$ and $f_s$ in dense samples ($D_{tc} = 66$ to 68%) for a $D_c/d_c = 25$. Wesley (2002) suggested an analytical procedure to estimate the percentage of correction required to correct cone tip resistances for $D_c/d_c$ ratios of 15, 25, 50 and 75. Accordingly, for a calibration chamber with $D_c/d_c$ ratio of 25, the maximum $q_c$ correction required for the current study, for tests at $D_{tc} = 65\%$, would be about 10% relative to measured $q_c$ values.

An infinite (very far) boundary in the field is neither BC1 nor BC3 as these boundary conditions simulate extreme limits of the most flexible and the most rigid boundaries. The actual in-situ boundary condition would be between BC1 and BC3 conditions, and probably somewhat closer to a BC5 condition (Huang and Hsu 2005; Goodarzi et al. 2018). Following the set of laboratory tests, an elaborate numerical study was conducted by simulating the physical calibration chamber and material properties to verify the influence of boundary conditions measured in CPT calibration chamber experiments and establish a detailed database of free-field penetration resistances determined through discrete element modeling.
2.3 Numerical DEM simulations

PFC3D from the Itasca Consulting Group Inc. (2002) is used to simulate DEM cone penetration tests. In PFC, the soil grains are modeled as sphere-shaped particles which interact at their contacts. There are three main steps in DEM simulation of a granular assembly: force exertion, disorder distribution and maintaining balance. At first, forces acting on particles are measured using a force-displacement law called the contact law. Afterward, particle positions are updated by Newton’s second law of motion. For a pseudo-static analysis, cycles continue until unbalanced forces acting on particles reach small amounts.

The rolling resistance contact model introduced in PFC was adopted in the present study. There are five different micromechanical parameters required to conduct a DEM simulation using this contact model including $E$ (modulus of elasticity of contacts), $k_{ratio}$ (shear to normal stiffness ratio among particle contact), $\mu$ (inter-particle friction), $\eta$ (inter-particle rolling resistance coefficient), and $\alpha_d$ (local damping coefficient). The magnitudes of these parameters were chosen and calibrated with the results of drained Direct Simple Shear (DSS) tests and odometer tests on loose and dense Boler sand performed by Mirbaha and Sadrekarimi (2017). As for the DSS samples, assemblies with 20000 spheres were generated in the domains of the sample with huge overlaps. The assembly is confined with two rigid highly frictional plates on top and bottom and 10 rigid rings in the peripheral position. After additional cycles to reduce the overlapping ratio, the samples are confined through the upper plate using a servo-mechanism. The final dimensions of the assemblies have a diameter of 70mm and a height of 20mm. The shearing is applied using a linear horizontal velocity distributed between the rings from 0 (top plate and its adjacent ring) to 0.1 mm/s (bottom plate and its adjacent ring). The velocity has been chosen low enough to reduce any dynamic effects. For the drained simulations used here, the servo-mechanism is maintained in the entire simulation. As for the Odometer simulations, the same assembly with similar dimensions is generated within the confines of a rigid frictionless cylinder. After minimizing the overlapping ratio, the assembly is confined to 50 kPa of initial pressure using a servomechanism applied on the upper plate. The e-logp' curve and the corresponding Normal Compression
Line (NCL) is obtained through a stress-controlled odometer simulation, while the void ratio of the sample is read using Representative Volume Elements (RVE)s embedded in the middle section of the sample. Similar approach has been used to estimate the relative densities of the DSS assemblies.

Elastic properties ($E, k_{ratio}$) of the particles were adjusted using the Normal Compression Line (NCL) obtained from odometric curve. Damping was set to 0.1 with a negligible effect as no dynamic effects exist in CPT. Inter-particle friction ($\mu$) and rolling resistance coefficient ($\eta$) were adjusted using the shear stress-strain curve of DSS test until the desired strength reached. That rolling resistance has negligible effect on the dilation angle of soil can be regarded as a persuasive tool to differentiate this parameter’s effect from inter-particle friction coefficient (Belheine et al. (2009)). Detailed discussion on the calibration procedure is further discussed by Alonso-Marroquin and Vardoulakis (2005), Gu et al. (2013).

Figure 2-5 shows that the stress-strain and volumetric behavior of the calibrated material and experimental tests compare favorably. Table 2-3 gives the calibrated parameters used in this study. To reduce the computational effort, the diameter of particles chosen for DEM simulations were scaled up by a factor of 9.
Figure 2-5: a) stress-strain, b) volumetric behavior and c) normal compression line (NCL) of calibrated DEM Direct Simple Shear and odometer tests and Experimental results performed by Mirbaha and Sadrekarimi (2017)

Figure 2-6 Schematics of the DEM-based (a) DSS specimen, (b) Odometer specimen
Table 2-3: Calibrated micromechanical parameters of the DEM simulation

<table>
<thead>
<tr>
<th>Micro material parameters</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle density (kg/m³), ( \rho )</td>
<td>2670</td>
</tr>
<tr>
<td>Modulus of elasticity of contact (MPa), ( E )</td>
<td>100</td>
</tr>
<tr>
<td>Normal to shear contact stiffness, ( k_{ratio} )</td>
<td>1.5</td>
</tr>
<tr>
<td>Inter-particle friction, ( \mu )</td>
<td>0.5</td>
</tr>
<tr>
<td>Inter-particle rolling coefficient, ( \eta )</td>
<td>0.4</td>
</tr>
<tr>
<td>Non-local damping coefficient, ( \alpha )</td>
<td>0.1</td>
</tr>
</tbody>
</table>

The specimen geometry adopted for the DEM simulations was a 100 mm high and 150 mm wide cylinder enclosed by two rigid boundaries on its top and bottom surfaces. The total number of particles were chosen to be 180000. The very large number of particles were used to minimize the amount of resonance among the particles, reduce the scaling effect, and produce smooth cone resistance profiles. This was further obtained by performing a series of simulations packed with different scaling factors. Figure 2-7 shows the variations of \( q_c \) for assemblies with different scaling factors. As can be seen, assemblies with lower scaling factors presented higher \( q_c \) values. Insignificant difference with less fluctuations is observed after scaling factor of 9, therefore it was chosen for the baseline simulations.
Initially, the particles were packed as a cloud of randomly overlapping particles within the sample domain and they were allowed to reach equilibrium while minimizing their overlap. They were then allowed to fall and settle by gravity and the sample was subjected to the specific boundary condition. Utilizing the multi-thread processing embedded into the new PFC6.0 version, this process took between 10 to 14 hours with an Intel® Core i9 9900k processor overclocked at 5 GHz. In constant stress boundary condition (BC1), stresses on the sample boundaries are controlled via a servomechanism. The lateral stress is defined as $K_0\sigma'_{vc}$, where $K_0$ is the lateral stress ratio found during consolidation of samples subjected to a BC3 boundary condition. For a laterally constrained ($\varepsilon_r = 0$) boundary condition (BC3), the specimen is modeled within a rigid cylinder and a constant $\sigma'_{vc}$ is applied by the servomechanism at the bottom of the sample. Finally, periodic boundaries are used to mimic infinite boundaries and minimize boundary effects close to the cone for a constant stiffness boundary condition (BC5), while applying confining stresses by a servo-controlled bottom wall. Reaching the required density and average mean stress, additional DEM cycles were embedded into the model to reduce the unbalanced forces and maintain a quasi-static regime in the system.
Figure 2-8 schematically illustrates the different boundary conditions applied to the particle assemblies in the DEM models.

Figure 2-8: Illustration of different boundary conditions applied in the DEM simulations

Samples of different packing densities were prepared by varying the inter-particle rolling coefficient (η) and inter-particle friction coefficient, (μ), from 0.05 to 0.5. A higher μ would resist particle rearrangement during deposition, holding particles apart and forming a porous fabric while lower μ would facilitate particle movement and forming denser particle packings. The initial void ratios of the samples were about 0.75, 0.69, 0.64 and 0.57 representing loose, medium dense, dense and very dense assemblies compared with e_{min} = 0.525 and e_{max} = 0.845 reported for Boler sand. The mentioned void ratio values were measured using the largest measurement circle confined in the boundaries of the simulated chamber. After consolidation and sample formation, the values of μ and η were set back to their calibrated values shown in Table 2-3. The cone penetrometer comprises a frictional cylindrical wall as the lower sleeve, a frictionless cylindrical wall as the upper sleeve and a rigid cone with an apex angle of 60°, 6 mm diameter and 5.2 mm height mounted at the top wall of the calibration chamber prior to cone penetration (Figure 2-9). The cone was then pushed into the sample at a constant velocity of 10 cm/s up to a depth of 6 cm. A higher penetration rate was used in the DEM simulations to reduce computational time, although penetration rate has no effect on q_c and f_s found in the DEM analyses. Different penetration rates showed no effect on the macroscale cone resistance results. To assess how far a system is from an equilibrium state, Index of Unbalanced
Forces ($I_{UF}$) is monitored as a relative indicator. Ng (2006b) introduced $I_{UF}$ to quantify the equilibrium state of an assembly of particles as below:

$$I_{UF} = \sqrt{\frac{\sum_{i=1}^{N}|F_i|^2/N}{\sum_{j=1}^{M}|F_j|^2/M}}$$  \hspace{1cm} [Eq. 1]

In which $I_{UF}$ is the index of unbalanced forces, $N$ and $M$ are the numbers of particles and contacts in the system, respectively, $|F_i|$ is the magnitude of the unbalanced force of particle $i$ and $|F_j|$ is the magnitude of the contact force of particle $j$ in the assembly. $I_{UF}$ was maintained below 0.01 for all simulations throughout penetration, which is a reasonable value according to Ng (2006b) representing a quasi-static granular system and therefore dynamic effects associated with inertial forces were negligible.

![Figure 2-9: Details of the cone and chamber cylinder used in this study](image)

Several CPT simulations were performed to investigate the effect of chamber height on the cone resistance response. Figure 2-10 presents the variations of $q_c$ with penetration depth for different chamber heights ranging from 10 to 17.5 cm. As shown in this figure,
chamber height has little effect on $q_c$ and therefore a chamber height of 10 cm was selected to reduce computational time for the rest of the CPT simulations.

![Figure 2-10: Variation of $q_c$ for different sample heights](image)

After finalizing the model parameters and constructing the samples, a series of CPT models were analyzed to study the effects of $D_{rc}$, $\sigma_{vc}$, and boundary conditions on the macro-scale responses of the cone. Table 2-4 summarizes test parameters used in these simulations.

<table>
<thead>
<tr>
<th>Test ID</th>
<th>$D_{rc}$ %</th>
<th>$e_c$</th>
<th>$\sigma_{vc}$ (kPa)</th>
<th>$K0$</th>
<th>$q_c$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BC1-L-50</td>
<td>27.5</td>
<td>0.757</td>
<td>50</td>
<td>0.540</td>
<td>4.72</td>
</tr>
<tr>
<td>BC1-L-100</td>
<td>26.5</td>
<td>0.760</td>
<td>100</td>
<td>0.540</td>
<td>6.17</td>
</tr>
<tr>
<td>BC1-L-200</td>
<td>27.5</td>
<td>0.750</td>
<td>200</td>
<td>0.524</td>
<td>7.69</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td></td>
</tr>
<tr>
<td>BC1-L-400</td>
<td>26.0</td>
<td>0.760</td>
<td>400</td>
<td>0.522</td>
<td>13.46</td>
</tr>
<tr>
<td>BC1-MD-50</td>
<td>48.7</td>
<td>0.689</td>
<td>50</td>
<td>0.540</td>
<td>7.62</td>
</tr>
<tr>
<td>BC1-MD-100</td>
<td>47.8</td>
<td>0.692</td>
<td>100</td>
<td>0.540</td>
<td>8.54</td>
</tr>
<tr>
<td>BC1-MD-200</td>
<td>48.1</td>
<td>0.690</td>
<td>200</td>
<td>0.523</td>
<td>11.03</td>
</tr>
<tr>
<td>BC1-MD-400</td>
<td>47.5</td>
<td>0.693</td>
<td>400</td>
<td>0.525</td>
<td>18.34</td>
</tr>
<tr>
<td>BC1-D-50</td>
<td>66.2</td>
<td>0.633</td>
<td>50</td>
<td>0.522</td>
<td>9.71</td>
</tr>
<tr>
<td>BC1-D-100</td>
<td>66.0</td>
<td>0.630</td>
<td>100</td>
<td>0.529</td>
<td>13.11</td>
</tr>
<tr>
<td>BC1-D-200</td>
<td>68.4</td>
<td>0.626</td>
<td>200</td>
<td>0.509</td>
<td>17.50</td>
</tr>
<tr>
<td>BC1-D-400</td>
<td>63.7</td>
<td>0.641</td>
<td>400</td>
<td>0.500</td>
<td>26.13</td>
</tr>
<tr>
<td>BC1-VD-50</td>
<td>85.9</td>
<td>0.570</td>
<td>50</td>
<td>0.490</td>
<td>13.01</td>
</tr>
<tr>
<td>BC1-VD-100</td>
<td>85.0</td>
<td>0.576</td>
<td>100</td>
<td>0.490</td>
<td>17.65</td>
</tr>
<tr>
<td>BC1-VD-200</td>
<td>84.0</td>
<td>0.576</td>
<td>200</td>
<td>0.480</td>
<td>25.81</td>
</tr>
<tr>
<td>BC1-VD-400</td>
<td>85.9</td>
<td>0.570</td>
<td>400</td>
<td>0.480</td>
<td>35.93</td>
</tr>
</tbody>
</table>

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>BC3-L-50</td>
<td>29.3</td>
<td>0.751</td>
<td>50</td>
<td>0.560</td>
</tr>
<tr>
<td>BC3-L-100</td>
<td>27.8</td>
<td>0.756</td>
<td>100</td>
<td>0.549</td>
</tr>
<tr>
<td>BC3-L-200</td>
<td>28.7</td>
<td>0.750</td>
<td>200</td>
<td>0.539</td>
</tr>
<tr>
<td>BC3-L-400</td>
<td>27.5</td>
<td>0.757</td>
<td>400</td>
<td>0.54</td>
</tr>
<tr>
<td>BC3-MD-50</td>
<td>48.4</td>
<td>0.690</td>
<td>50</td>
<td>0.565</td>
</tr>
<tr>
<td>BC3-MD-100</td>
<td>47.5</td>
<td>0.693</td>
<td>100</td>
<td>0.546</td>
</tr>
<tr>
<td></td>
<td>Column 1</td>
<td>Column 2</td>
<td>Column 3</td>
<td>Column 4</td>
</tr>
<tr>
<td>----------------</td>
<td>----------</td>
<td>----------</td>
<td>----------</td>
<td>----------</td>
</tr>
<tr>
<td>BC3-MD-200</td>
<td>46.2</td>
<td>0.697</td>
<td>200</td>
<td>0.540</td>
</tr>
<tr>
<td>BC3-MD-400</td>
<td>45.3</td>
<td>0.700</td>
<td>400</td>
<td>0.531</td>
</tr>
<tr>
<td>BC3-D-50</td>
<td>64.0</td>
<td>0.640</td>
<td>50</td>
<td>0.547</td>
</tr>
<tr>
<td>BC3-D-100</td>
<td>62.8</td>
<td>0.644</td>
<td>100</td>
<td>0.540</td>
</tr>
<tr>
<td>BC3-D-200</td>
<td>65.3</td>
<td>0.636</td>
<td>200</td>
<td>0.520</td>
</tr>
<tr>
<td>BC3-D-400</td>
<td>62.8</td>
<td>0.628</td>
<td>400</td>
<td>0.516</td>
</tr>
<tr>
<td>BC3-VD-50</td>
<td>83.4</td>
<td>0.578</td>
<td>50</td>
<td>0.520</td>
</tr>
<tr>
<td>BC3-VD-100</td>
<td>85.9</td>
<td>0.570</td>
<td>100</td>
<td>0.520</td>
</tr>
<tr>
<td>BC3-VD-200</td>
<td>86.8</td>
<td>0.567</td>
<td>200</td>
<td>0.518</td>
</tr>
<tr>
<td>BC3-VD-400</td>
<td>89.6</td>
<td>0.558</td>
<td>400</td>
<td>0.510</td>
</tr>
<tr>
<td>BC5-L-50</td>
<td>24.6</td>
<td>0.766</td>
<td>50</td>
<td>0.540</td>
</tr>
<tr>
<td>BC5-L-100</td>
<td>26.8</td>
<td>0.759</td>
<td>100</td>
<td>0.540</td>
</tr>
<tr>
<td>BC5-L-200</td>
<td>28.7</td>
<td>0.753</td>
<td>200</td>
<td>0.531</td>
</tr>
<tr>
<td>BC5-L-400</td>
<td>29.6</td>
<td>0.750</td>
<td>400</td>
<td>0.540</td>
</tr>
<tr>
<td><strong>BC5</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BC5-MD-50</td>
<td>49.3</td>
<td>0.687</td>
<td>50</td>
<td>0.552</td>
</tr>
<tr>
<td>BC5-MD-100</td>
<td>49.0</td>
<td>0.680</td>
<td>100</td>
<td>0.550</td>
</tr>
<tr>
<td>BC5-MD-200</td>
<td>49.3</td>
<td>0.697</td>
<td>200</td>
<td>0.533</td>
</tr>
<tr>
<td>BC5-MD-400</td>
<td>44.0</td>
<td>0.703</td>
<td>400</td>
<td>0.530</td>
</tr>
<tr>
<td>BC5-D-50</td>
<td>61.8</td>
<td>0.647</td>
<td>50</td>
<td>0.530</td>
</tr>
</tbody>
</table>
2.4 Results and discussions

2.4.1 Model validation and preliminary results

Figure 2-11 compares the variations of $q_c$ with $D_{rc}$ from the DEM simulations with those measured in the CPT experiments of this study for different boundary conditions. As illustrated in this figure, $q_c$ computed from the DEM simulations compare favorably with those measured in the laboratory calibration chamber experiments at all $D_{rc}$ and $\sigma'$ values. Figure 2-12 demonstrates the profiles of $q_c$ with cone penetration depth for different $D_{rc}$ and boundary conditions. For the sake of brevity, only the results of $\sigma'_{vc} = 400\text{kPa}$ are presented. Irrespective of the boundary condition, $q_c$ increases with increasing $D_{rc}$ and penetration depth. While the scaled-up gradation used in the CPT models has resulted in some fluctuations in $q_c$, a plateau is reached after a penetration depth of about 4 cm. Accordingly, the average cone tip resistance from a penetration depth of 4 to 6 cm is taken as the ultimate $q_c$ mobilized in each simulation.
Figure 2-11: Comparisons of average $q_c$ determined in the DEM simulations with those measured in the calibration chamber experiments (a) BC1, (b) BC3
Figure 2-12: Profiles of $q_c$ at $\sigma'_{ve} = 400$ kPa for different $D_{rc}$ and a) BC1, b) BC3, and c) BC5 boundary conditions
2.4.2 Effect of $D_{rc}$ and $\sigma'_{vc}$

To highlight the effect of radial boundary condition, the profiles of $q_c$ for BC1, BC3, and BC5 boundary conditions are compared in Figure 2-13. Similar to the CPT calibration chamber tests, comparatively higher $q_c$ is ultimately mobilized in BC3 conditions than those under BC1 conditions. Higher $q_c$ values obtained in chambers with rigid boundaries have also been achieved by Butlanska et al. (2014b) and Salgado et al. (1998) through simulating calibration chambers using DEM and FEM, respectively. Cone tip resistances produced in samples subjected to a BC5 condition are between those mobilized under BC3 and BC1 conditions. Similar trend is also reported by Goodarzi et al. (2018) in finite element analysis of CPT with different boundary conditions.
Emphasizing the effect of $D_{rc}$ on lateral boundary effects, Figure 2-14 depicts the obtained $q_c$ values with different initial states. It can be inferred that in all tests, the boundary effect reduces as the relative density reaches values lower than 45% (medium-dense to loose sand). Furthermore, with decreasing confining pressure, boundary effects amplify at a given relative density.

Figure 2-15 demonstrates the effect of $\sigma'_{vc}$ on $q_c$, which has been normalized by a reference pressure of $P_a = 100$ kPa. As expected, the values of $q_{cN} = q_c/P_a$ increase with increasing $\sigma'_{vc}/P_a$ for both chamber tests and DEM simulations. These trends for chamber test and simulation results are fitted with power functions in Figure 2-15 and compare favorably for various relative densities. The boundary condition effect is also visible herein, showing an increase for BC3 boundary condition compared to stress-controlled radial boundaries of BC1 and BC5. Similar to Figure 2-14, the effect of boundary condition is absent at $D_{rc} = 25\%$ and appears for $D_{rc} \geq 45\%$ in Figure 2-15. The significance of boundary effect also increases with decreasing $\sigma'_{vc}$.
Figure 2-14: Comparisons of $q_c$ for different boundary conditions and $D_{rc}$ for $\sigma'_{vc}$ of a) 400 kPa, b) 200 kPa, c) 100 kPa and d) 50 kPa

Figure 2-15: Effect of $\sigma'_{vc}$ on $q_c$ for different boundary conditions and $D_{rc}$

Table 2-5 and Table 2-6 present the total and the relative increases in $q_c$ from BC1 to respectively BC3 and BC5 boundary conditions. The relative changes present an increase of up to 21% at $D_{rc} = 85\%$ and $\sigma'_{vc} = 50\text{kPa}$. 
Table 2-5: Total and relative (%) increases in $q_c$ from a BC1 to a BC5 boundary condition based on DEM simulations

<table>
<thead>
<tr>
<th></th>
<th>50 kPa</th>
<th>100 kPa</th>
<th>200 kPa</th>
<th>400 kPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loose ($D_{rc} = 25%$)</td>
<td>0.37 (7.8%)</td>
<td>0.21</td>
<td>0.22</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td>(3.4%)</td>
<td>(2.9%)</td>
<td>(1.2%)</td>
<td></td>
</tr>
<tr>
<td>Medium dense ($D_{rc} = 45%$)</td>
<td>0.73 (10.1%)</td>
<td>0.46</td>
<td>0.48</td>
<td>0.56 (3%)</td>
</tr>
<tr>
<td></td>
<td>(5.4%)</td>
<td>(4.3%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dense ($D_{rc} = 65%$)</td>
<td>1.61 (16.5%)</td>
<td>1.67 (12.7%)</td>
<td>1.76 (10%)</td>
<td>2.34 (8.9%)</td>
</tr>
<tr>
<td>Very dense ($D_{rc} = 85%$)</td>
<td>2.78 (21.3%)</td>
<td>2.63 (14.9%)</td>
<td>3.18 (12.3%)</td>
<td>3.89 (10.8%)</td>
</tr>
</tbody>
</table>

Table 2-6: Total and relative (%) increases in $q_c$ from a BC1 to a BC3 boundary condition from DEM simulations

<table>
<thead>
<tr>
<th></th>
<th>50 kPa</th>
<th>100 kPa</th>
<th>200 kPa</th>
<th>400 kPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loose ($D_{rc} = 25%$)</td>
<td>0.43 (9.2%)</td>
<td>0.36</td>
<td>0.31</td>
<td>0.32</td>
</tr>
<tr>
<td></td>
<td>(5.9%)</td>
<td>(4.1%)</td>
<td>(2.4%)</td>
<td></td>
</tr>
<tr>
<td>Medium dense ($D_{rc} = 45%$)</td>
<td>0.93 (12.8%)</td>
<td>0.68</td>
<td>0.75</td>
<td>0.78</td>
</tr>
<tr>
<td></td>
<td>(7.9%)</td>
<td>(6.8%)</td>
<td>(4.2%)</td>
<td></td>
</tr>
<tr>
<td>Dense ($D_{rc} = 65%$)</td>
<td>1.84 (19%)</td>
<td>2.14 (16.3%)</td>
<td>2.43 (13.9%)</td>
<td>3.01 (11.5%)</td>
</tr>
<tr>
<td>Very dense ($D_{rc} = 85%$)</td>
<td>3.47 (26.7%)</td>
<td>3.18 (18%)</td>
<td>4.05 (15.7%)</td>
<td>5 (13.9%)</td>
</tr>
</tbody>
</table>
2.4.3 Radial stress changes

To better explain the difference in $q_c$, both the micro and the macro behaviors are examined. To this end, several RVEs (Representative Volume Elements) were added to the model along the axis of penetration in the centerline. Each RVE is a sphere with a radius of 10 mm ($20d_{50}$) involving almost 1500 particles and records the macro and micro scale parameters. Figure 2-16 to 2-19 show the variations of radial stress ($\sigma_r$) normalized by $\sigma'_vc$, measured by the REV spheres in samples under various $\sigma'_vc$ and $D_{rc}$ before penetration. The effect of fixed radial boundary (BC3) is marked here with values of $\sigma_r/\sigma'_vc$ above those observed in BC1 and BC5 boundary conditions for all simulations. This effect reduces at lower relative densities ($D_{rc}=25-45\%$). Several studies (Baldi et al. 1981; Hunstman, 1985; Salgado et al. 1998) show that $q_c$ is highly affected by the horizontal effective stress than $\sigma'_vc$. Accordingly, the larger $q_c$ mobilized in BC3 conditions in Figure 2-13 can be associated with the higher $\sigma_r$ developed for this boundary condition. Similar to $q_c$ in Figure 2-13, the difference in $\sigma_r/\sigma'_vc$ between different boundary conditions reduces with increasing $\sigma'_vc$. This likely the result of reduced dilatancy and more contractive behavior of sand at higher stress levels.

![Diagram](a) ![Diagram](b)
Figure 2-16: Variations of normalized radial stress with normalized penetration depth for samples consolidated to $\sigma'_{vc}$ of a) 50kPa, b) 100kPa, c) 200kPa and d) 400kPa at 25% relative density.
Figure 2-17 Variations of normalized radial stress with normalized penetration depth for samples consolidated to $\sigma'_{vc}$ of a) 50kPa, b) 100kPa, c) 200kPa and d) 400kPa at 45% relative density.
Figure 2-18 Variations of normalized radial stress with normalized penetration depth for samples consolidated to $\sigma'_vc$ of a) 50kPa, b) 100kPa, c) 200kPa and d) 400kPa at 65% relative density.
Figure 2-19 Variations of normalized radial stress with normalized penetration depth for samples consolidated to $\sigma'_vc$ of a) 50kPa, b) 100kPa, c) 200kPa and d) 400kPa at 85% relative density

2.4.4 Force chain and displacement fields

Concerning the particle scale observations, Figure 2-20, Figure 2-21 and Figure 2-22 illustrate the strong contact force chains and particle displacements in assemblies with different confinements and relative densities. The thickness of the lines in force chain distributions represents the magnitude of each contact force. The contact forces with magnitudes less than 50 N are eliminated for better illustration. Concentrated around the cone in all assemblies, a qualitative trend can be achieved. The distribution of strong contact force chains is more pronounced in assemblies with higher relative densities and confinement in all boundary conditions. As can be seen in all figures, the thickness and distribution of strong force chains are more intensified for BC3 and BC5 boundary condition. Similar trend is observed in different boundary conditions and confinement stresses. This agrees with higher radial stresses observed in those boundary conditions in 2.4.3. Regarding the displacement fields, it can be observed that smaller number of particles close to the cone shaft are entrapped in the large displacement field for BC1 samples compared to BC3 and BC5. Similar trend is captured in various confinements and relative densities.
Figure 2-20: Strong force chain distribution and particle displacements at the end of penetration in loose assemblies (D_{rc}=25\% \text{ and } \sigma'_{vc}=100 \text{ kPa}) with (a) BC1, (b) BC3 and BC5 boundary conditions
Figure 2-21: Strong force chain distribution and particle displacements at the end of penetration in very dense assemblies ($D_\text{rc}=85\%$ and $\sigma'_\text{vc}=100$ kPa) with (a) BC1, (b) BC3 and BC5 boundary conditions
Figure 2-22: Strong force chain distribution and particle displacements at the end of penetration in loose assemblies ($D_{rc}=25\%$ and $\sigma'_{vc}=400$ kPa) with (a) BC1, (b) BC3 and BC5 boundary conditions.
2.4.5 Correction for boundary effect

As discussed above, the effect of different boundary conditions depends on both $D_{rc}$ and $\sigma'_{vc}$. Using BC5 as the benchmark, a correction factor (CF) is proposed for converting $q_c$ from BC1 and BC3 conditions to the corresponding free-field values as below:

$$q_{cc} = q_{cb} \times CF$$  \hspace{1cm} \text{[Eq. 2]}

Where $q_{cc}$ is the corrected $q_c$ corresponding to free-field conditions with no boundaries, and $q_{cb}$ is $q_c$ measured under BC1 and BC3 boundary conditions. Figure 2-23 depicts the variations of the proposed correction factor with $\sigma'_{vc}$ at different $D_{rc}$. These trends are fitted with the following function:

$$CF = a \left( \frac{\sigma'_{vc}}{P_a} \right)^b + c D_{rc}^d$$  \hspace{1cm} \text{[Eq. 3]}

The above correlation is proposed to determine the free-field $q_c$ from calibration chamber tests conducted with BC1 and BC3 boundary conditions, respectively. The factors have a value: $a = 1.03$, $b = -0.031$, $c = 0.00015$ and $d = 1.51$ for BC1 boundary condition and $a = 0.992$, $b = 0.0031$, $c = -0.00044$ and $d = 0.91$ for BC3 boundary condition.
Figure 2-23: Variations of CF with $\sigma'_v/P_a$ at different $D_{rc}$ for (a) BC1 and (b) BC3 boundary conditions

2.4.6 Comparison with other studies

Figure 2-24 shows the comparison of correction factor values according to various prepositions for $D_{rc} = 65\%$. The correction factor obtained from DEM simulations shows a favorable agreement with the propositions of Wesley (2002a).
Figure 2-24: The correction coefficient based on various propositions and DEM for BC1 experiments with Drc=45 and 65%
2.5 Conclusion

In the present research, the variations of cone tip and sleeve frictional resistances in different boundary conditions were investigated using DEM simulations and laboratory calibration chamber experiments. Favorable quantitative agreement was captured between numerical and experimental results. As observed in both DEM and calibration chamber tests, stress-controlled boundary condition (BC1) provides lower $q_c$ values compared to BC3 boundary condition. This effect amplifies with relative density and dissipates with vertical stress of the assembly; however, little influence of boundary condition was confirmed by DEM and experimental tests for loose and medium dense ($D_r=25\%$ and 45\%) samples. Similarly, an average increase of 24\% is noticed for sleeve frictional resistances from BC1 to BC3 condition in laboratory tests; however, the sleeve friction variation has been disregarded in DEM simulations due to significant resonance in the results. The variation of normalized radial stress measured by RVEs situated at the axis of penetration in DEM simulations shows that the boundary effect observed in denser assemblies is attributed to the appreciable difference in lateral pressure distribution along the cone axis. Furthermore, correction factors were proposed considering BC5 boundary condition as a benchmark for free-field cone resistance, with a better agreement with the predictions of Wesley (2002b).
Chapter 3

3 Comprehensive Study on the Effect of Microparameters on CPT Measurements

A clear perspective on the effect of various micro parameters gives an insight into the test data interpretation and soil behavior. For this purpose, this chapter describes the application Discrete Element Method to simulate cone penetration test. Influence of state, stress history, microparameters (e.g. modulus, rolling resistance, interparticle friction and probe interface friction), particle shape (angularity) and probe geometry are investigated on tip resistance and sleeve friction measurements.

3.1 Introduction

Geotechnical design projects require accurate site characterization, soil stratigraphy, and strength parameters. In-situ assessment of these parameters is of utmost importance specifically in cohesionless soils from which taking undisturbed samples seem an onerous task (Yoshimi et al. (1978)). Therefore, many attempts have been made to correlate between the parameters obtained in in-situ tests and design parameters of soils (e.g., Schmertmann (1978a), Jamiolkowski et al. (2003)). The Cone Penetration Test (CPT) is an in-situ testing method that is widely used to characterize the subsurface soil and obtain its geotechnical parameters. In CPT, the soil properties are obtained indirectly from the soil response to the penetration. It has become one of the most popular testing methods due to its repeatability, rapidity, and accuracy. However, conducting in-situ CPT for research purposes could be challenging. Therefore, numerous attempts have been made to investigate the cone penetration in laboratory-scale tests namely calibration chambers (Schmertmann (1978b), Villet and Mitchell (1981), Parkin and Lunne (1982), Jamiolkowski et al. (1985), Been et al. (1987)). Calibration chambers often contain large quantities of soil and suffer from inhomogeneity in the soil medium Ghionna and Jamiolkowski (1991). Miniature Cone Penetration Tests (MCPT), an alternative to the problematic size of calibration chambers, also present notable boundary and scale effects. For this purpose, researchers have used analytical (Vesic (1972), Janbu and Senneset (1974), Durgunoglu and Mitchell (1975), Salgado et al. (1997), Yu (2000)) and numerical
approaches (Baligh (1985), Teh and Houlsby (1991), Sagaseta et al. (1997), Abu-Farsakh et al. (1998), Lu et al. (2004), Ahmadi and Robertson (2005), Moug et al. (2016), Gupta et al. (2016)) to investigate the mechanism of cone penetration test. Concerning the analytical approaches, the dilatant behavior of sand during shearing has not been accounted and they are only valid in loose-medium dense sands. Furthermore, the large-deformation nature of penetration problems generates the necessity of complex constitutive models or adaptive remeshing techniques (Jiang et al. (2006a), Butlanska et al. (2014b)).

The aforementioned techniques utilize the continuum-based approximations that are incapable of delineating the true distinct nature of coarse-grain soils. Capturing this trait, Discrete Element Method (DEM) has widespread popularity among engineers in modeling granular assemblies and geotechnical problems concerning large deformation. DEM was first proposed by Cundall and Strack (1979) as a tool for modeling interaction between rigid blocks of rock. Many attempts (Huang et al. (1993), Nova (2005), Jiang et al. (2006a), Lin and Wu (2012), Butlanska et al. (2014a), Falagush et al. (2015a), Ciantia et al. (2016), Khosravi et al. (2019), Peters et al. (2019)) have been conducted to simulate CPT in granular assemblies using DEM. Huang et al. (1993) were probably the first to use DEM to simulate penetration problems. They used a combined Discrete Element Method-Boundary Element Method (DEM-BEM) to simulate the penetration of cone in sand in plane strain condition. Their results show that both the penetration mechanism and soil dilatancy in a granular material are affected by its loading history. Jiang et al. (2006b) used a 2D-DEM model focusing on soil-cone interface friction. It was observed that the cone resistance increases with increasing depth and tip-soil friction coefficient. High gradients of particle rotation, particle displacements and velocity fields were observed around the cone tip throughout the penetration. In the same vein, Jiang et al. (2014) studied the mechanism of inclined CPT in granular ground using DEM. Several penetration tests were carried out with different inclination angles with respect to the ground surface. It was observed that the normalized tip resistance \( q_c = q_c / \sigma_v \) increases with inclination angle. Nova (2005) simulated 2D-DEM models of cone penetration and biaxial compression tests targeting the effect of confinement and initial porosity on the macroscopic parameters. Although plane strain simulations presented satisfactory
qualitative trends, they are incapable of representing the actual behavior of granular media due to differences in contact geometry and porosity calculations (Falagush et al. (2015a)).

Arroyo et al. (2011) simulated a virtual calibration chamber using 3D-DEM model. The contact model was calibrated using drained triaxial results on Ticino sand. Particle rotation was prohibited to account for particle angularity and non-sphericity. The ratio of chamber diameter to cone diameter ($D_c/d_c$) is 16.9 and grain size scaling of 50 was used in the study. The results of tests with shorter cone diameter exhibited large oscillations due to the short cone diameter to grain average diameter ratio ($d_c/D_{50}$). Although quantitative agreement was obtained with experimental results of CPT on Ticino sand, particle size scaling used could have affected the responses at micro level. Butlanska et al. (2009) studied the effect of radial walls on the homogeneity of the specimen previously studied by Arroyo et al. (2011). Frictionless radial walls were introduced to benefit from the symmetry of the penetration problem and reduce the number of particles in each simulation. It was observed that reducing the chamber section size tends to increase the cone resistance.

Falagush et al. (2015a) simulated a 30° calibration chamber using 3D-DEM modeling. A particle refinement method was applied to model sand size particles next to the cone. Isotropic boundary condition has been applied using cylindrical and top walls. It has been observed that prohibiting particle rotation increases the cone resistance significantly. Falagush et al. (2015a) used different particle shapes using the clump technic and found out that particle shape has a pronounced effect on cone resistance. Additionally, particle crushing was included, which was found to influence the tip resistance.

Lin and Wu (2012) studied the influence of cone geometry on $q_c$ and $f_s$ using DEM. A miniature calibration chamber was modeled and compacted using boundary contraction and servo walls. Radial walls were embedded within the confines of the model to benefit from the axisymmetric nature of the CPT. It was successfully observed that reducing the cone diameter increases the cone resistance and sleeve friction.
Syed et al. (2017) in another study investigated the effect of soil relative density using a 3D-DEM model calibration chamber. After calibration of micro parameters using Hertz-Mindlin contact model, three penetration tests on loose, medium, and dense sand were carried out and compared with experimental results. Their model compared favorably with experiments only within the range of 5-30% soil relative density.

Khosravi et al. (2019) attempted to investigate the influence of inter-particle and wall-particle interface characteristics on CPT measurements. 3D-DEM based virtual calibration chambers (VCCs) were modeled with 70 cm diameter, $D_c/d_c = 15.9$ and $d_c/D_{50} = 3.1$. $K_0$ and isotropic consolidated ($\sigma'_v = 100$ kPa) assemblies were simulated using boundary contraction method to model the behavior of poorly-graded Ottawa 20-30 sand. The parametric study on CPT measurements presented that inter-particle friction and rolling resistance have strong influence on cone tip resistance and a milder effect on sleeve friction. Moreover, probe-particle friction coefficient was found to have a significant influence on $f_s$, with negligible effect on $q_c$ values. Although valuable insights were obtained on the effect of micro parameters in this study, the performed simulations were confined to a limited series of relative densities and vertical pressures, with no regard for elastic parameters.

Kotrocz and Kerényi (2019) investigated the effect of inter-particle DEM contact properties on the cone resistance using a 3D calibration chamber. After particle generation, gravity was applied to the particles, allowing them to settle until a pseudo-static equilibrium is reached. Afterward, the bonding between the particles was applied to simulate a cohesive soil. It was concluded that parallel bond radius, particle shear modulus and stiffness affect the results significantly. On the other hand, particle density and Poisson-ratio have negligible effect on the penetration resistance.

Ostensibly, most studies modeling calibration chambers encounter substantial boundary effects, limiting the choice of $D_c/d_c$ ratios in their simulations. Furthermore, gradual erosion and deface occurring to the probe due to frequent testing has been neglected in the previous research. Precise choice of elastic and strength parameters is necessary to obtain realistic CPT measurements and soil classifications, especially when accounting
for the dilative behavior of coarse-grained soils. Therefore, within the confines of this paper, it is attempted to comprehensively investigate the influence of micro-parameters (particle-particle and probe-particle) on CPT measurements ($q_c$ and $f_s$) at various relative densities and vertical stresses. The goal is to determine a realistic insight into the particulate assembly state properties and modeling parameters used in DEM simulation of CPT in a free-field setting.

3.2 Numerical DEM simulations

3.2.1 Calibration of microparameters

PFC3D from the Itasca Consulting Group Inc. (2002) is used to simulate DEM cone penetration tests. Although a non-linear formulation (Hertz-Mindlin) might best describe the force-displacement response, it is computationally expensive and does not yield significant difference (Di Renzo and Di Maio (2004)). Therefore, the computationally efficient rolling resistance linear ($rrlinear$) model is chosen as a built-in contact model that applies the effect of particle shape into the general linear contact model. To calibrate the micro parameters for this study, a series of Drained Direct Simple Shear Tests (DSS) and Odometer tests were simulated and compared with the so-called Fraser River Sand (FRS). Three sets of DSS tests with relative densities of 30, 40 and 46% with different confinement pressures were modelled and compared with numerical DSS tests. The compressibility of the sample was verified by modeling uniaxial compression simulations on loose ($D_{rc}=6\%$) assemblies. Figure 3-1 shows the particle size distribution (PSD) curve of the Fraser river sand used in this study.
As for the DSS test, the model consists of an assembly confined with 10 rigid rings with a diameter of 7cm and thickness of 0.2cm, generating a cylindrical prism with 2 cm height. The walls of the sample were modeled as frictionless. The baseline for comparison in this section is the DSS tests conducted by Jones (2017) on FRS. The scaled-up particle assembly (scaling factor of $N = 3$) is constructed with 10000 spherical particles and a gradation similar to the Fraser river sand PSD curve. No contribution in the force chains is observed for particle sizes less than $d_{10}$ in the analyses (Lin and Wu (2012), Hazeghian and Soroush (2015), Chang et al. (2015)); therefore, these particles were omitted before the compaction stage in both DSS and odometer simulations. The particle assembly is generated within the domain of the test as a packed assembly with overlaps. DEM cycles are performed to minimize the overlaps and maintain balance within the system. Then, the sample is consolidated using the stress-controlled top platen. To achieve an assembly with the required densities, particle friction coefficient ($\mu$) is varies between 0.1 to 0.5 to change the interlock between particles and generate different void ratios. This parameter was changed to its actual value at the shearing stage. The initial void ratio of the sample
after consolidation ($e_c$) is recorded using the measurement spheres embedded into the model. Shearing is applied by giving a strain rate to the bottom plate and the rings in the horizontal direction, varying linearly between 0.1 mm/s for the bottom plate to 0 mm/s for the upper plate. A constant stress was maintained during shearing on the top platen to achieve a drained simulation condition. The details of the DEM-DSS testing is presented in chapter 4.

As for the odometer tests, a rigid cylinder with frictionless walls was modeled and filled with 8000 spheres (scaling factor of $N = 3.5$). The particles with gradation similar to that of FRS were generated at random positions with overlaps. The geometry of the odometer at 5 kPa equilibrium state for all simulations is characterized by a diameter of 70 mm and a height of 21 mm. After performing enough cycles to minimize the overlaps, the particles settled by applying gravity. A stress-controlled mechanism with a maximum speed of 0.01 m/s was applied to the assembly through the top wall while the volumetric strain of the sample was recorded simultaneously. To achieve a loose assembly, both $\mu$ and $\eta$ were applied in the sample generation stage to maximize the particle interlocks and increase the void ratios. The variations of void ratios were carefully monitored through three main Representative Volume Elements (RVE)s embedded along the depth of the assembly. Simulations were performed using different values of effective modulus ($E$) to capture the corresponding modulus of elasticity of FRS obtained by tests performed by Jones (2017). The details of the DSS and Odometer simulation conditions are presented in Table 3-1.
### Table 3-1 DSS and Odometer simulation characteristics

<table>
<thead>
<tr>
<th>Parameters</th>
<th>DEM-DSS</th>
<th>DEM-Odometer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample height ((H))</td>
<td>20mm</td>
<td>21mm</td>
</tr>
<tr>
<td>Sample diameter ((D))</td>
<td>70mm</td>
<td>70mm</td>
</tr>
<tr>
<td>Scaling factor ((N))</td>
<td>3</td>
<td>3.5</td>
</tr>
<tr>
<td>Number of spheres</td>
<td>10000</td>
<td>8000</td>
</tr>
<tr>
<td>loading rate (max)</td>
<td>0.1mm/s</td>
<td>0.01 m/s</td>
</tr>
<tr>
<td>Boundary condition</td>
<td>rigid</td>
<td>rigid</td>
</tr>
<tr>
<td>Particle shape used</td>
<td>sphere</td>
<td>sphere</td>
</tr>
</tbody>
</table>
Figure 3-2: Schematics of a) DSS and b) odometer samples modeled for calibration using DEM

Two sets of parameters are mainly applied in the used contact model. Elastic parameters (e.g., effective modulus $E$, normal to shear stiffness ratio $k_{ratio}$) whose values mainly affect the initial slope of the stress-strain curve of the sample, and rupture parameters (e.g., inter-particle friction coefficient $\mu$, $\eta$) that affect the friction angle, strength or the material and volumetric behavior. First, the micro parameters are chosen and varied until a satisfactory agreement is achieved in the stress-strain-volumetric behavior curves of the assembly; afterward, the macro parameters of the DEM assembly and experiments are compared. Comprehensive details of the calibration process are further explained by Gu et al. (2013). The validity of the rolling resistance can be further calibrated with the concept of angle of repose. A series of numerical analysis coupled with simple experiment were performed to calibrate the values of $\eta$ to match the angle of repose of
the DEM assemblies with experiment. In both cases, the particles are poured from a conical helix through gravity on a flat surface, resulting in a pile with a specific surface angle. If the surface angle exceeds $\phi'_{cs}$, the slipping begins in the mantle of the assembly. Figure 3-3 illustrates the results of the funnel analysis for various rolling resistances compared with the repose angle of FRS. As depicted in this picture, the angle of repose increases with increasing rolling resistance.

![Funnel analysis test for assemblies with different η values and results](image)

**Figure 3-3: Funnel analysis test for assemblies with different η values and results; a) FRS, b) η=0.0, c) η=0.4, d) η=0.6**

Figure 3-4a and Figure 3-4b present the stress-strain and volumetric behavior of the adopted assemblies and FRS obtained in DSS simulations. Favorable agreement is obtained between the experimental numerical tests. Figure 3-4c presents the variation of the coefficient of compressibility in terms of axial stress obtained from odometer tests and simulations. The chosen effective modulus compares favorably with the value of 100
MPa. Table 3-2 presents the final micro parameters calibrated for the baseline simulation for CPT tests in the present study.

![Graphs showing stress-strain, volumetric behavior, and coefficient of compressibility](image)

**Figure 3-4:** a) stress-strain, b) volumetric behavior and c) coefficient of compressibility of calibrated DEM DSS and odometer tests and Experimental results
Table 3-2: Calibrated micromechanical parameters of the DEM simulation

<table>
<thead>
<tr>
<th>Micro material parameters</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle density (kg/m$^3$), $\rho$</td>
<td>2690</td>
</tr>
<tr>
<td>Modulus of elasticity of contact (MPa), $E$</td>
<td>100</td>
</tr>
<tr>
<td>Normal to shear contact stiffness, $k_{ratio}$</td>
<td>1.5</td>
</tr>
<tr>
<td>Inter-particle friction, $\mu$</td>
<td>0.7</td>
</tr>
<tr>
<td>Inter-particle rolling coefficient, $\eta$</td>
<td>0.4</td>
</tr>
<tr>
<td>Non-local damping coefficient, $\alpha$</td>
<td>0.1</td>
</tr>
</tbody>
</table>

3.2.2 DEM modeling methodology to simulate CPT

The specimen geometry adopted for the CPT tests is a cube with dimensions of 280mm×280mm×350mm enclosed with two rigid walls on top and bottom. A total of 250000 particles with gradation similar to that of Fraser river sand with scaled dimensions constitute the model assembly. Particles finer than D$_{10}$ were eliminated from the assembly as they do not contribute to the force chain network and increase the runtimes significantly. A similar practice has been performed by Lin and Wu (2012), Hazeghian and Soroush (2015), Chang et al. (2015) to minimize the computational effort in their simulations. A series of simulations on loose (D$_{rc}$=25%) and very dense (D$_{rc}$=85%) assemblies are performed to investigate the effect of fine particles on CPT measurements. As illustrated in Figure 3-5, insignificant difference is observed between the normalized $qc$ and $fs$ profiles after omitting finer particles.
Figure 3-5: Influence of particles finer than $D_{10}$ in loose and very dense DEM assemblies reflected in terms of a) normalized $q_c$ and b) normalized $f_s$. 

(a) 

(b)
The application of periodic boundaries in these simulations was to eliminate the boundary effect. Such boundaries allow particles to pass from the parallelepiped domain to a fictitious adjacent one and simulate an infinitely periodic (repeated) system in the lateral direction (El Shamy and Zamani (2012)). Using high number of particles reduces the resonance in the cone resistance results and omits the scaling effect. The particle packings were prepared using the “multi-layer under compaction” method introduced by Jiang et al. (2003). In this method, first, the required number of particles (50000 spheres at each stage) are produced randomly within the boundary of the system. Afterward, the rigid boundaries were loaded by a rate-controlled mechanism to consolidate the specimen to the desired state with void ratio values higher than those required after consolidation. Then, the under-compaction method is applied again for different layers with decreasing void ratios to achieve a homogenous sample. The detailed study on the sample preparation can be found in Jiang et al. (2003). Finally, the heightened gravity of 200g similar to centrifuge modeling was applied to the particles and the top wall was eliminated from the model. Additional cycles were imbedded into the model to reduce the unbalanced forces and maintain a quasi-static regime in the system. This process took between 12 to 18 hours with an Intel® Core i9 9900k processor overclocked at 5 GHz. It should be noted that the inter-particle friction coefficient, $\mu$, was chosen from values between 0.05-1 during the preparation stage to achieve assemblies with different relative densities. Inter-particle rolling was also considered during the packing phase to increase the void ratio of the system in loose assemblies. As for the penetration stage, the values of the inter-particle friction coefficient and rolling resistance coefficient were set back to their calibrated values for the baseline simulation. The compound effect of these two parameters generates assemblies with four different void ratios of 0.876, 0.804, 0.738 and 0.678 representing loose, medium dense, dense and very dense assemblies. The void ratio of the sample is measured using the average of three large measurement spheres (RVE) imbedded along the depth and five RVEs along the width of the model in x and y directions. These RVEs have 30% of overlap in each direction. Figure 3-6 presents the variation of void ratios along with the depth of the assemblies with different relative densities (solid bullets) compared with the average void ratio measured from the major
RVE inside the sample (dashed lines). It can be observed that the state of the assemblies is quite homogeneous in all cases and depths.

![Graph showing variation of void ratios along the depth of the assemblies compared with the average void ratio measured from major RVE](image)

**Figure 3-6**: variation of void ratios along the depth of the assemblies compared with the average void ratio measured from major RVE

The probe mounted directly on top of the soil assembly consists of a frictionless conic with 60° apex angle and 10 cm² surface area for $q_c$ measurements, a frictional cylinder with 134mm height for $f_s$ measurements, and a frictionless cylinder. Keeping the rest of the parameters the same, the ball-probe modulus is chosen 1000 times higher than the ball-ball modulus in the simulations. Actual dimensions of the CPT based on ASTM D5778 have been chosen to be more comparable to the field tests.
The tip resistance \( q_c \) measurements are recorded as the vertical response of the frictionless cone divided by the area of the cone and sleeve friction \( f_s \) measurements are recorded as the vertical response of the frictional sleeve divided by the area of the sleeve. The probe penetrates through the assembly with a heightened rate of 20 cm/s to reduce the runtimes. To optimize the computational cost, a series of preliminary tests were performed on loose calibrated material with penetration rates of 0.02, 0.05, 0.1, 0.2 and 0.5 m/s. To assess whether the system remains in an equilibrium state, Index of Unbalanced Forces \( (I_{UF}) \) has been recorded throughout the penetration as:

\[
I_{UF} = \sqrt{\frac{\sum_{i=1}^{N} |F_i|^2}{N}} \cdot \frac{\sqrt{\sum_{j=1}^{M} |F_j|^2}}{M}
\]

[Eq. 1]
Where $I_{UF}$ is the index of unbalanced forces, $N$ and $M$ are the numbers of particles and contacts in the system, respectively, $|F_i|$ is the magnitude of the unbalanced force of particle $i$ and $|F_j^c|$ is the magnitude of the contact force of particle $j$ in the assembly. For the calculation cycles, automatic timestep calculation ($1-1.2 \times 10^{-6}$) has been chosen for the CPT simulations based on critical timestep of the system.

According to Figure 3-8, The values of $I_{UF}$ were reported to be lower than 0.01 in all simulations with rates below 0.2 m/s, representing a quasi-static state with insignificant dynamic effects for tests according to Ng (2006a), while dynamic effects begin to appear for penetration rates above 0.5 m/s.
Figure 3-8: Influence of penetration rate in loose DEM assemblies reflected in terms of a) normalized $q_c$ and b) normalized $f_s$.

DEM matrix calculations are sensitive to the hardware and software update and alterations. For this reason, a series of simulations of loose ($D_{re}=25\%$) and very dense ($D_{re}=85\%$) assemblies are performed to verify the repeatability of the results. As illustrated in Figure 3-9, the DEM results are perfectly repeatable.
Figure 3-9: Repeatability analysis for loose and very dense DEM assemblies reflected in terms of a) normalized $q_c$ and b) normalized $f_s$. 

\begin{itemize}
  \item $E = 100\,\text{MPa}$
  \item $\mu = 0.7$
  \item $\eta = 0.4$
  \item $k_{\text{ratio}} = 1.5$
  \item $D_{\text{rc}} = 85\%$
  \item $D_{\text{rc}} = 25\%$
\end{itemize}
3.2.3 Fundamental aspects of the DEM granular assembly

To better understand the characteristics of the soil assembly, a triangular velocity of 0.02 m/s was applied to the rigid bedrock for 3ms. The model was then allowed to oscillate freely while recording the time required for the free vibration of the system. The shearing strain was small enough to be in the linear range. Figure 3-10 presents the time history of the average particle velocity at different stress levels. For the sake of brevity, the results of the loose assembly are only presented. This history is corresponding to an average low strain shear wave velocity of 160 m/s or low strain shear modulus of 36 MPa, representing a loose granular deposit. The distance between the base and the measurement circles divided by the time to present the first peak in the time history is calculated as low strain shear wave velocity. Figure 3-11 demonstrates the variation of shear wave velocities in terms of normalized vertical pressure ($\sigma'_v/P_a$) for assemblies with different relative densities. The results of the shear wave velocity measurements are summarized in Table 3-3.
Figure 3-10: Time history of the average particle velocity at different stress levels for the loose assembly caused by an impulse loading.
Figure 3-11: Variation of low strain shear wave velocities in terms of normalized vertical pressure for assemblies with different relative densities
Table 3-3 Summary of the \( V_s \) measurements

<table>
<thead>
<tr>
<th>( D_{10} ) (%)</th>
<th>( \sigma'_{vc} ) (kPa)</th>
<th>Travel distance (cm)</th>
<th>Arrival time (s)</th>
<th>( V_s ) (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25%</td>
<td>49.9</td>
<td>28.86</td>
<td>0.0024</td>
<td>116</td>
</tr>
<tr>
<td></td>
<td>97</td>
<td>24.86</td>
<td>0.0017</td>
<td>143.5</td>
</tr>
<tr>
<td></td>
<td>196.2</td>
<td>17.19</td>
<td>0.001</td>
<td>166.57</td>
</tr>
<tr>
<td></td>
<td>405</td>
<td>13.69</td>
<td>0.00064</td>
<td>214</td>
</tr>
<tr>
<td>47%</td>
<td>54.8</td>
<td>29.28</td>
<td>0.0021</td>
<td>134.33</td>
</tr>
<tr>
<td></td>
<td>102</td>
<td>25.59</td>
<td>0.0015</td>
<td>160.75</td>
</tr>
<tr>
<td></td>
<td>203</td>
<td>21.08</td>
<td>0.001</td>
<td>193.88</td>
</tr>
<tr>
<td></td>
<td>402</td>
<td>15.38</td>
<td>0.00064</td>
<td>240.37</td>
</tr>
<tr>
<td>67%</td>
<td>54</td>
<td>27.49</td>
<td>0.0017</td>
<td>158.4</td>
</tr>
<tr>
<td></td>
<td>96</td>
<td>24.35</td>
<td>0.0013</td>
<td>181.7</td>
</tr>
<tr>
<td></td>
<td>199</td>
<td>22.85</td>
<td>0.00099</td>
<td>231.2</td>
</tr>
<tr>
<td></td>
<td>400</td>
<td>18.61</td>
<td>0.00068</td>
<td>273.7</td>
</tr>
<tr>
<td>85%</td>
<td>50</td>
<td>26.8</td>
<td>0.0014</td>
<td>186.4</td>
</tr>
<tr>
<td></td>
<td>101</td>
<td>25.27</td>
<td>0.001</td>
<td>235.33</td>
</tr>
<tr>
<td></td>
<td>198</td>
<td>21.79</td>
<td>0.0008</td>
<td>272.44</td>
</tr>
<tr>
<td></td>
<td>401</td>
<td>15.88</td>
<td>0.00048</td>
<td>331</td>
</tr>
</tbody>
</table>
Figure 3-12 presents the variations of horizontal stress, vertical stress and the coefficient of pressure at rest (K0) along the depth of the assemblies with various relative densities. The stress fields are calculated using the RVEs embedded along the depth of the sample. Each RVE has a diameter of 20$d_{50}$ and includes about 3000 spheres. As observed, the vertical and horizontal stresses increase linearly with the depth. A slight non-linearity at the end of the sample could be attributed to the boundary effect of the bottom plate. It is observed that the coefficient of pressure at rest first decreases and then asymptotically reach a constant value. Satisfactory agreement is captured between the K0 obtained from RVEs and the values obtained from the empirical method presented by Jaky. J (1944). Similar observations in variations of K0 were reported by Jiang et al. (2015a) in 2D simulations of DEM assemblies.
Figure 3-12: Variations of horizontal stress, vertical stress and coefficient of pressure at rest (K0) for assemblies with a) $D_{rc}=25\%$, b) $D_{rc}=47\%$, c) $D_{rc}=67\%$ and d) $D_{rc}=85\%$

The behavior of the DEM assemblies for different relative densities in terms of normalized parameters (for $q_{c1N}$ and $f_{s1N}$) is plotted in Figure 3-13. According to the classification proposed by Robertson (2016), the DEM assemblies data drop in the areas with “sand mixtures” to “clean sand” labels. According to the examples of soils provided in Robertson (2016), the classification of the DEM assemblies ($Q_{tn} = 32$ and $F_r = 0.6$) is consistent with normally consolidated sandy tailings and normally consolidated sand deposits.
Figure 3-13: Soil behavior type chart of the modeled assemblies in different relative densities according to Robertson (2016)

3.2.4 Problem description and test series

A series of Cone Penetration tests were performed to study the effect of various parameters on the macro scale response of the test. Table 3-4 gives a summary of test conditions including particle size, relative density, effective modulus ($E^*$), inter-particle friction coefficient ($\mu$), inter-particle rolling resistance ($\eta$), particle shape (A.R), geometry of the probe including cone angle and combined cone and sleeve friction coefficients. Analysis with model parameters of $E^*=100\text{MPa}$, $\mu=0.7$, $\eta =0.4$, A.R=1, cone angle of 60°, cone friction coefficient of 0.0 and sleeve friction coefficient of 0.5 has been chosen as the benchmark for comparison with other simulations. Considering the effect of particle size, the analyses are denoted as Drati where i takes values of 1 to 4. As for the effect of relative density, the analyses are denoted as Dri where i takes values of 25, 47, 67 and 85 representing the corresponding relative density percentage of the proposed analyses. Simulations with the ID of OCRi are performed to investigate the effect of
stress history and over-consolidation ratio (OCR) on CPT measurements where i represents the OCR of the assembly. Tests with the ID of Ei are performed to investigate the effect of effective modulus on macroscale responses where i takes values of 50, 100, 150 and 200 representing the corresponding effective modulus in MPa for the proposed analyses. To investigate the effect of particle surface roughness, tests denoted as PFi-(L or D) were performed where i takes values of 0.7, 0.6, 0.5, 0.4, 0.2 and 0.05 representing the interparticle friction coefficient used in the analyses. To account for the influence of particle shape, two approaches were chosen: 1) In A.Ri (L or D) analyses, the actual shape of the particles is modeled using clump logic with i taking values of 1, 1.5 and 2 as the particle aspect ratio. 2) In RRi (L or D) analyses the effect of particle shape is accounted using rolling resistance coefficient applied between spherical particles in all directions where i takes values of 0.0, 0.2, 0.3, 0.4 and inhibited rolling. As for the effect of probe geometry, the analyses are donated as CAi- (L or D) where i takes values of 45°, 60°, 90°- and 120°-degrees representing cone angle used in simulations. The compound effect of cone-sleeve friction coefficient is performed in analyses with ID CiSj-(L, MD, D and VD) where i and j take values of 0.0, 0.25 and 0.5 as the coefficient of friction used for the facets in simulations. The notations of L, MD, D, and VD set for analyses id represent the state of the simulation as Loose, Medium Dense, Dense, and Very Dense, respectively. In the present study, the effect of the abovementioned parameters is investigated on the variations of cone resistance ($q_c$) and sleeve friction ($f_s$) and Soil Behavior Type classifications (SBT) charts provided by Robertson (2016).
<table>
<thead>
<tr>
<th>Test No.</th>
<th>Aim</th>
<th>Drc %</th>
<th>$e_c$</th>
<th>OCR</th>
<th>$D_r/D_{50}$</th>
<th>Effective modulus, $E^*$ (MPa)</th>
<th>particle friction coefficient, $\mu$</th>
<th>Rolling resistance friction coefficient, $\eta$</th>
<th>A.R</th>
<th>Cone angle °</th>
<th>Cone friction coefficient</th>
<th>Sleeve friction coefficient</th>
<th>$I_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drat1</td>
<td>To study the effect of particle size on $q_c$ and $f_s$</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>2.3</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>-</td>
</tr>
<tr>
<td>Drat2</td>
<td></td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>-</td>
</tr>
<tr>
<td>Drat3</td>
<td></td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>5.75</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>-</td>
</tr>
<tr>
<td>Drat4</td>
<td></td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>8</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>-</td>
</tr>
<tr>
<td>Dr25</td>
<td>To study the effect of different soil relative densities on $q_c$ and $f_s$</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>2.03</td>
</tr>
<tr>
<td>Dr45</td>
<td></td>
<td>47</td>
<td>0.80</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>1.90</td>
</tr>
<tr>
<td>Dr65</td>
<td></td>
<td>67</td>
<td>0.73</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>1.89</td>
</tr>
<tr>
<td>Dr85</td>
<td></td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>1.81</td>
</tr>
</tbody>
</table>
To study the effect of over consolidation stress on $q_c$ and $f_s$,

| OCR1  | 25 | 0.87 | 1 | 3.45 | 100 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 2.03 |
| OCR2  | 25 | 0.87 | 2 | 3.45 | 100 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 1.91 |
| OCR4  | 25 | 0.87 | 4 | 3.45 | 100 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 1.84 |
| OCR8  | 25 | 0.87 | 8 | 3.45 | 100 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 1.80 |
| OCR16 | 25 | 0.87 | 16 | 3.45 | 100 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 1.78 |

| E50-L | 25 | 0.87 | 1 | 3.45 | 50  | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 2.06 |
| E100-L| 25 | 0.87 | 1 | 3.45 | 100 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 2.03 |
| E150-L| 25 | 0.87 | 1 | 3.45 | 150 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 1.92 |
| E200-L| 25 | 0.87 | 1 | 3.45 | 200 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 1.89 |
| E50-VD| 85 | 0.67 | 1 | 3.45 | 50  | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 1.81 |
| E100-VD| 85 | 0.67 | 1 | 3.45 | 100 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 1.82 |
| E150-VD| 85 | 0.67 | 1 | 3.45 | 150 | 0.7 | 0.4 | 1 | 60° | 0 | 0.5 | 1.70 |
To study the effect of different particle friction coefficients on $q_c$ and $f_s$, representing grain roughness.

<table>
<thead>
<tr>
<th>Friction Coefficient</th>
<th>$q_c$ (mm)</th>
<th>$f_s$</th>
<th>$v_d$ (m/s)</th>
<th>$\theta$ (deg)</th>
<th>$h$ (m)</th>
<th>$\phi$ (deg)</th>
<th>$r_f$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PF0.7-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>1</td>
</tr>
<tr>
<td>PF0.6-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.6</td>
<td>1</td>
</tr>
<tr>
<td>PF0.5-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.5</td>
<td>1</td>
</tr>
<tr>
<td>PF0.4-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.4</td>
<td>1</td>
</tr>
<tr>
<td>PF0.2-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.2</td>
<td>1</td>
</tr>
<tr>
<td>PF0.05-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.05</td>
<td>1</td>
</tr>
<tr>
<td>PF0.7-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>1</td>
</tr>
<tr>
<td>PF0.6-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.6</td>
<td>1</td>
</tr>
<tr>
<td>PF0.5-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.5</td>
<td>1</td>
</tr>
<tr>
<td>PF0.4-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.4</td>
<td>1</td>
</tr>
<tr>
<td>PF0.2-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.2</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>------</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>PF0.05-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.05</td>
<td>0.4</td>
</tr>
<tr>
<td>RR0.4-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
</tr>
<tr>
<td>RR0.3-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.3</td>
</tr>
<tr>
<td>RR0.2-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.2</td>
</tr>
<tr>
<td>RR0.1-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.0</td>
</tr>
<tr>
<td>RR0.4-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
</tr>
<tr>
<td>RR0.3-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.3</td>
</tr>
<tr>
<td>RR0.2-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.2</td>
</tr>
<tr>
<td>RR0.0-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.0</td>
</tr>
<tr>
<td>AR1-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.0</td>
</tr>
<tr>
<td>AR1.5-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.0</td>
</tr>
</tbody>
</table>

To study the effect of different particle rolling resistance coefficients on $\eta_c$ and $f_s$, representing grain angularity.

To study the effect of different particle aspect.
<table>
<thead>
<tr>
<th>AR2-L</th>
<th>25</th>
<th>0.87</th>
<th>1</th>
<th>3.45</th>
<th>100</th>
<th>0.7</th>
<th>0.0</th>
<th>2</th>
<th>60°</th>
<th>0</th>
<th>0.5</th>
<th>2.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>AR2-MD</td>
<td>25</td>
<td>0.80</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.0</td>
<td>2</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>1.89</td>
</tr>
<tr>
<td>AR2-D</td>
<td>25</td>
<td>0.73</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.0</td>
<td>2</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>1.68</td>
</tr>
<tr>
<td>AR1-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.0</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>2.23</td>
</tr>
<tr>
<td>AR1.5-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.0</td>
<td>1.5</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>1.78</td>
</tr>
<tr>
<td>AR2-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.0</td>
<td>2</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>1.74</td>
</tr>
<tr>
<td>CA45-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>45°</td>
<td>0</td>
<td>0.5</td>
<td>2.31</td>
</tr>
<tr>
<td>CA60-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>2.03</td>
</tr>
<tr>
<td>CA90-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>90°</td>
<td>0</td>
<td>0.5</td>
<td>1.76</td>
</tr>
<tr>
<td>CA120-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>120°</td>
<td>0</td>
<td>0.5</td>
<td>1.64</td>
</tr>
<tr>
<td>CA45-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>45°</td>
<td>0</td>
<td>0.5</td>
<td>1.96</td>
</tr>
</tbody>
</table>

To study the effect of different cone angles on qc and fs.
<table>
<thead>
<tr>
<th></th>
<th>25</th>
<th>0.87</th>
<th>1</th>
<th>3.45</th>
<th>100</th>
<th>0.7</th>
<th>0.4</th>
<th>1</th>
<th>60°</th>
<th>0</th>
<th>0.5</th>
<th>1.94</th>
</tr>
</thead>
<tbody>
<tr>
<td>CA60-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>60°</td>
<td>0</td>
<td>0.5</td>
<td>1.82</td>
</tr>
<tr>
<td>CA90-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>90°</td>
<td>0</td>
<td>0.5</td>
<td>1.53</td>
</tr>
<tr>
<td>CA120-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
<td>1</td>
<td>120°</td>
<td>0</td>
<td>0.5</td>
<td>1.38</td>
</tr>
</tbody>
</table>

To study the effect of combined cone & sleeve friction coefficients on $q_c$ and $f_s$, representing cone erosion over time.
<table>
<thead>
<tr>
<th>Table Entry</th>
<th>CF0.0-VD</th>
<th>CF0.25-VD</th>
<th>CF0.5-VD</th>
<th>CSF0.0-L</th>
<th>CSF0.0-MD</th>
<th>CSF0.0-D</th>
<th>CSF0.0-VD</th>
</tr>
</thead>
<tbody>
<tr>
<td>CF0.0-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
</tr>
<tr>
<td>CF0.25-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
</tr>
<tr>
<td>CF0.5-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
</tr>
<tr>
<td>CSF0.0-L</td>
<td>25</td>
<td>0.87</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
</tr>
<tr>
<td>CSF0.0-MD</td>
<td>47</td>
<td>0.80</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
</tr>
<tr>
<td>CSF0.0-D</td>
<td>67</td>
<td>0.73</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
</tr>
<tr>
<td>CSF0.0-VD</td>
<td>85</td>
<td>0.67</td>
<td>1</td>
<td>3.45</td>
<td>100</td>
<td>0.7</td>
<td>0.4</td>
</tr>
</tbody>
</table>
3.3 Results and discussions

3.3.1 Effect of particle size

To achieve a uniform sample with reasonable computational effort, various samples were made with different scaling factors to investigate the effect of $D_c/D_{50}$ on $q_c$ and $f_s$. $D_c/D_{50}$ ratios of 8, 5.75, 3.45 and 2.3 were generated corresponding to loose assemblies ($D_e=25\%$) with 398400, 250000, 120800 and 51500 spheres, respectively. Figure 3-14 illustrates the variations of normalized cone resistance ($q_{cN}$) and normalized sleeve friction ($f_{sN}$) for assemblies with different $D_c/D_{50}$ ratios. As can be seen, significant oscillations occur in profiles with lower $D_c/D_{50}$ ratios. This is due to lower resulted contacts from particles touching the probe. It is observed that increasing the particle size increases both cone and frictional sleeve resistances, with higher influence on $f_{sN}$. Similar observations were reported by Butlanska et al. (2014a), Khosravi et al. (2019) by simulation of calibration chambers using DEM. Samples with 250000 and 398400 spheres presented similar $q_{cN}$ and $f_{sN}$ profiles; therefore, $D_c/D_{50}$ ratio of 5.75 is chosen for the baseline simulations in this study.

The variations of normalized shear wave velocities for assemblies with different $D_c/D_{50}$ ratio is illustrated in Figure 3-15. As can be seen, with increasing the particle size, the normalized shear wave velocity increases until $D_c/D_{50}$ ratio of 5.75. 28.5% difference is captured between assemblies with 51500 and 250000 particles. Insignificant difference is observed between assemblies with $D_c/D_{50}$ ratios of 5.75 and 8.
Figure 3-14: variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration of the assemblies with different $D_c/D_{50}$ ratios.

Figure 3-15 Variation of normalized shear wave velocity for assemblies with different particle sizes ($D_c/D_{50}$).
3.3.2 Effect of relative density

Figure 3-16a and Figure 3-16b illustrate the variations of normalized cone tip resistance (\(q_{cN} = q_c/P_a\)) and normalized sleeve friction resistance (\(f_{sN} = f_s/P_a\)) for assemblies with various relative densities, respectively. Regarding the values of minimum and maximum void ratios reported by Jones (2017) as \(e_{\text{min}} = 0.63\) and \(e_{\text{max}} = 0.96\), the obtained void ratios of 0.876, 0.804, 0.738 and 0.678 capture relative densities of 25%, 47%, 67% and 85%, respectively. It can be observed that both \(q_c\) and \(f_s\) increase throughout the penetration. This progression is in agreement with those observed in centrifuge modeling of CPT (Bolton et al. (1999)). The penetration measurements do not change significantly at the beginning of the penetration until the cone and sleeve become fully activated and enough number of particles surround the probe along with penetration. It is further highlighted that both \(q_c\) and \(f_s\) increase significantly with relative density. Higher relative density is associated with higher mean effective stress generated around the probe (Lunne (1997)), leading to higher \(q_c\), \(f_s\) and shear strength of the soil. Figure 3-16c and d present the variation of \(q_{cN}\) and \(f_{sN}\) over normalized effective vertical stress for assemblies with different relative densities. Similar to void ratio measurements, the variations of vertical stress along the depth of the sample are computed using the average value of all vertical stresses in each RVE stress tensor. The trends of the \(q_{cN}\) and \(f_{sN}\) variations are in agreement with the results of calibration chamber tests performed on Fraser River Sand reported by Jones (2017), where both parameters increase with increasing \(D_{rc}\) and vertical stress.

Often estimating the sleeve friction (\(f_s\)) from \(q_c\) values is of interest to the engineers as different cone designs engender less reliable \(f_s\) results (Lunne et al. (1988)). For this purpose, Figure 3-16d presents the correlation between normalized cone tip resistance and normalized sleeve frictional resistance at 100 kPa vertical stress. With increasing relative density, both \(q_c\) and \(f_s\) increase linearly in DEM simulations, shown in Equation 1:

\[
q_{c1N} = 59.323f_{s1N} + 37.921 \quad (R^2 = 0.987) 
\]

[Eq. 1]
Concerning the SBT classification, the obtained normalized values of cone resistance and sleeve friction at 100 kPa vertical pressure are plotted to study the effect of state at penetration problems. Hereafter, the notations in the classification charts denote as SD: sand like- dilative, SC: sand like- contractive, TD: transitional-dilative, TC: transitional-contractive, CD: clay like- dilative, CC: clay like- contractive, CCS: clay like-contractive-sensitive. The corresponding values of the state parameter (ψ) for each test are provided in the graph. These values are obtained using a comparison between the void ratios of the assemblies and critical state line (CSL) of Fraser River Sand studied by Jones (2017). It can be observed that the data series move towards the upper right side of the graph, from sand with slightly contractive behavior (ψ = 0.0185 for Drc=25%) to sand with complete dilative behavior (ψ = -0.2115 for Drc=85%).

Obtaining undisturbed samples from granular soils is an onerous task (Yoshimi et al. (1978), Hatanaka et al. (1988), Goto et al. (1992)). Therefore, it is of interest to the geotechnical engineers to estimate the in-situ relative density of the soil using penetration tests. Figure 3-17 illustrates the correlation of Drc and qc1N obtained from DEM simulations. The specific correlation developed from this study is given as:

\[ D_{rc} (\%) = 51.563 \ln(q_{c1N}) - 182.32\ (R^2 = 0.97) \]  

[Eq. 2]

Most of the test series are performed at Drc=25% and 85% in this study. For the sake of brevity, only a few supplementary simulations were performed at Drc=47% and 67% to complete this plot for the effect of various parameters, while assuming a logarithmic trend between Drc-qc1N.

Several studies (Baldi et al. 1981; Hunstman, 1985; Salgado et al. 1998) show that qc is highly affected by the horizontal effective stress than σve. For this reason, the variations of normalized qc and fs over normalized effective horizontal stress for assemblies with different relative densities is presented in Figure 3-18. Similar to the vertical stress, the values of the horizontal stress are measured using RVEs embedded along with the depth of the model. σ'xx or σ'y and σ'zz from the stress tensor represent the values for horizontal and vertical stresses, respectively. As can be seen, a steeper slope is observed for both qc1N
and $f_{sN}$ compared to their corresponding values on vertical stress in Figure 3-16c and Figure 3-16d.
Figure 3-16: variation of a) $q_{CN}$ in terms of relative penetration, b) $f_{SN}$ in terms of relative penetration, c) $q_{CN}$ in terms of normalized vertical pressure, d) $f_{SN}$ in terms of normalized vertical pressure, e) $q_{c1N}$ in terms of $f_{s1N}$ and f) SBT classification (Robertson (2016)) of the assemblies with different relative densities
Figure 3-17: $D_{rc}$ and $q_{c1N}$ correlation obtained from DEM simulation for Fraser River Sand

Figure 3-18: Variations of a) $q_{cN}$ on normalized horizontal pressure and b) $f_{sN}$ on normalized horizontal pressure in different relative densities
To illustrate the progressive localization in CPT, void ratio distributions were captured using RVEs in the post-processing stage. Grids of measurement spheres are located around the cone with distance to measure the void ratios and read the locus of the center of the sphere (Figure 3-19). Due to symmetry of the problem, only a limited cube of the sample was probed in x-z plane for post-processing.

Figure 3-20 and Figure 3-21 illustrate the contours of void ratio distributions obtained from RVEs before and after penetration. As can be seen, the assemblies are homogeneous in both loose and very dense assemblies after consolidation. A quantitative agreement is achieved between the contour distribution and void ratio measurements from Major RVEs for loose and very dense assemblies (e=0.876 and 0.678). In the deep penetration ($z/r=10$), localized areas with high void ratios generate along the length of the probe. The diameter of the localized area is about $4D_c$ in areas near the surface. The values of the void ratio distribution demonstrate that active areas generate beneath the cone, while passive areas are located before the cone along the frictional sleeve with higher values of void ratios.
Figure 3-19: Systematic grids of RVEs for porosity calculation and post-processing
Figure 3-20: Void ratio distribution obtained in post processing for loose assembly in a) after consolidation b) after deep penetration

Figure 3-21: Void ratio distribution obtained in post processing for very dense assembly in a) after consolidation b) after deep penetration
Particle size measurements culminate invaluable insights into the penetration mechanism. Figure 3-22 illustrates the accumulated particle displacements at the end of penetration for assemblies with different relative densities. As can be seen, the particles displace as high as 10 cm along with the probe penetration. This volume of localized deformation is spread up to $4d_{50}$ at each side of the cone. Accordingly, a heave at both sides of the probe is observed on the free air surface. Figure 3-23 presents the distribution of particle velocities at the end of penetration for assemblies with different relative densities. The maximum velocity field is observed around the cone for each assembly. The velocity field observed for both cases is more consistent with the failure mechanism predicted by Berezantev and Vesic for deep penetration. This localized failure can be seen in terms of force chain distributions in Figure 3-24. The thickness of the lines represents the magnitude of each contact force. The contact forces with magnitudes less than 100 N are eliminated for better illustration. As can be seen, the strong contact force chains are concentrated around the cone for all assemblies. The distribution of strong contact force chains is more concentrated around the probe in assemblies with higher relative densities, leading to higher reaction and increased $q_c$ and $f_s$ measurements.
Figure 3-22: Distribution of particle displacements at the end of penetration for (a) $D_{rc}=25\%$, (b) $D_{rc}=47\%$, (c) $D_{rc}=67\%$ and (d) $D_{rc}=85\%$
Figure 3-23: Distribution of particle velocity at the end of penetration for (a) $D_{rc}=25\%$, (b) $D_{rc}=47\%$, (c) $D_{rc}=67\%$ and (d) $D_{rc}=85\%$
Figure 3-24: Strong contact force chain map distribution at the end of penetration for (a) $D_{rc}=25\%$, (b) $D_{rc}=47\%$, (c) $D_{rc}=67\%$ and (d) $D_{rc}=85\%$
3.3.3 Effect of stress history

Over-consolidation effect is an important factor in studying liquefaction susceptibility using CPT (Roy et al. (2019)). To investigate the effect of stress history on CPT measurements, a series of CPTs were performed on loose ($D_{rc}=25\%$) assemblies with different over-consolidation ratios (OCR). After consolidation, a higher gravitational field was applied to the assemblies and particles were allowed to reach equilibrium with additional cycles. Before the start of penetration, the values of the gravity were set back to 200g to achieve over-consolidation ratios of 2, 4, 8, and 16.

Figure 3-25a and Figure 3-25b illustrate the influence of OCR on $q_{cN}$ and $f_{sN}$ profiles. As observed, both cone and sleeve resistances are highly influenced by the stress history. A 100% increase in $q_{cN}$ profile is observed for OCR=16. Similar observations regarding increase in cone tip resistance were reported by Roy et al. (2019) while performing CPT in a centrifuge chamber. Figure 3-25c presents the variation of $q_{cN}$ over normalized effective vertical stress for assemblies with different OCR values. It is demonstrated that $q_{cN}$ increases with increasing normalized vertical stress for assemblies with various stress histories. This trend is amplified for higher values of OCR and is presented in Figure 3-25d. Figure 3-25e depicts the SBT classification of simulations with various OCR levels. A shift towards the upper right side of the plot is observed with increasing OCR, leading to a more dilative response.

Concerning the particle-scale measurements, Figure 3-26 shows the distribution of particle displacements at the end of penetration for assemblies with different over consolidation ratios. As can be seen, the extent of the zone with large particle displacements increase with increasing the OCR in assemblies. Figure 3-27 illustrates the distribution of the strong contact force map distributions at the end of penetration for assemblies with different over consolidation ratios. The contact forces with magnitudes less than 100 N are eliminated for better illustration. It can be observed that with increasing OCR, larger contact forces are mobilized along the probe, the majority of which are concentrated around the cone.
(a) $q_{cN} = q_c/P_a$

(b) $f_{sN} = f_s/P_a$

(c) $q'_{cN} = q_c/P_a$

(d) OCR

(e) $Q_o$

(f) $V_s$ (m/s)
Figure 3-25: variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) normalized $q_c$ in terms of normalized vertical pressure, d) $q_{cN}$ in terms of OCR e) SBT classification and f) normalized shear wave velocity variation of the assemblies with different over-consolidation ratios (OCR)

The variations of normalized shear wave velocities for assemblies with different over consolidation ratios is illustrated in Figure 3-25f. As can be seen, with increasing the OCR, $V_{S1}$ increases. 35% increase is observed between the assemblies with OCR levels of 16 and normally consolidated sample.
Figure 3-26: Distribution of particle displacements in loose assemblies at the end of penetration with (a) OCR=1, (b) OCR=2, (c) OCR=4, (d) OCR=8 and (e) OCR=16
Figure 3-27: Strong contact force chain map distribution in loose assemblies at the end of penetration with (a) OCR=1, (b) OCR=2, (c) OCR=4, (d) OCR=8 and (e) OCR=16
3.3.4 Effect of effective modulus ($E^*$)

Rolling resistance model in PFC uses a soft contact approach where all deformation occurs at contacts between discrete rigid bodies; As a result, the stiffnesses can be related to the effective modulus ($k_n ~ E^*$) of an equivalent continuum (Potyondy (2018)). Several studies (Combarros et al. n.d., Zhou et al. (1999), (2001), Landry et al. (2006), Coetzee et al. (2010), Lommen et al. (2013), Yohannes et al. (2014), Coetzee (2017)) have been performed on the effect of elastic parameters on the behavior of granular materials using DEM. Despite some discrepancies, most studies generally indicate that at low stiffness (linear or nonlinear) values, macro response of the material such as internal friction angle and cohesion is affected and after a certain limit, the effect of stiffness dissipates. However, it should be noted that a choice of low modulus might lead to huge particle overlaps, contradictory to the basic Discrete Element Method assumptions (O’Sullivan (2011)). Lommen et al. (2013) investigated the effect of shear modulus ($G$) on penetration test results using Hertz-Mindlin contact model. Penetration resistance increased from 11 to 14 MPa for $G = 10^7$-$10^9$ Pa and only half of that increase was observed for $G=10^4$-$10^6$ Pa. Kotrocz and Kerényi (2019), through performing a series of 3D-DEM simulations, reported an increase of penetration resistance with shear modulus, though negligible effects on tip resistance were observed after $G=4*10^7$ Pa.

Using a linear DEM formulation, simulations were performed in this study on assemblies with different effective moduli ($E^*$). Figure 3-28a and Figure 3-28b illustrate the variations of $q_{cN}$ and $f_{sN}$ in terms of relative penetration for the mentioned simulations. It is observed that effective modulus does not have a significant effect on CPT measurements. A 100% increase in effective modulus from 50 to 100 MPa results in 22.3% and 35% increase in $q_{cN}$ for $D_r=25\%$ and $D_r=85\%$, respectively (Figure 3-28d). Figure 3-28c presents $q_{cN}$ over normalized vertical stress for loose and very dense DEM assemblies. As observed, $E^*$ does not play a significant role at lower normalized pressures; however, this effect highlights with increasing vertical pressure up to 400 kPa. The act of grain compressibility is unclear in higher pressures as particle crushing has not been considered in this discussion. Figure 3-28e depicts the SBT classification of
simulations performed on samples with various moduli. The effective modulus does not change the soil behavior, irrespective of the soil relative density.

Figure 3-29 illustrates the variations of small-strain shear wave velocities on normalized effective vertical stress and the variation of shear wave velocities at 100 kPa vertical pressure for assemblies with various effective modulus. The modulus is changed after consolidation and S-wave is generated through the bedrock to be received via RVEs. As can be seen, Vs increases with increasing the effective modulus for both loose and very dense assemblies. This increase amplifies in higher confinement stresses. However, smaller difference is observed at $D_{rc}=85\%$ for the different values of $E^*$. It can be concluded that higher compressibility leads to lower shear wave velocities in granular assemblies.

Regarding the particle-scale measurements, Figure 3-30 and Figure 3-31 show the distribution of particle displacements at the end of penetration for loose and very dense assemblies with different effective modulus. As can be seen, effective modulus does not have a significant influence on the displacement magnitudes. Figure 3-32 and Figure 3-33 illustrate the distribution of the strong contact force map distributions at the end of penetration for loose and very dense assemblies with different effective modulus. The contact forces with magnitudes less than 100 N are eliminated for better illustration. As illustrated, increasing the effective modulus leads to stronger and more scattered normal contact forces mobilized along the probe. The extent of the zone with strong contact forces is larger in very dense assemblies.
Figure 3-28: variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) normalized $q_c$ in terms of normalized vertical pressure, d) $q_{c1N}$ in terms of $f_{s1N}$ and e) SBT classification of the assemblies with different $E^*$
Figure 3-29: Shear wave velocity measurements for packings with different effective moduli ($E^*$) at loose and very dense relative densities.
Figure 3-30: Distribution of particle displacements at the end of penetration in loose assemblies for (a) E=50MPa, (b) E=100MPa, (c) E=150MPa and (d) E=200MPa
Figure 3-31: Distribution of particle displacements at the end of penetration in very dense assemblies for (a) $E=50\text{MPa}$, (b) $E=100\text{MPa}$, (c) $E=150\text{MPa}$ and (d) $E=200\text{MPa}$
Figure 3-32: Strong contact force chain map distribution at the end of penetration in loose assemblies for (a) $E=50$MPa, (b) $E=100$MPa, (c) $E=150$MPa and (d) $E=200$MPa
Figure 3.33: Strong contact force chain map distribution at the end of penetration in very dense assemblies: (a) $E=50\text{MPa}$, (b) $E=100\text{MPa}$, (c) $E=150\text{MPa}$ and (d) $E=200\text{MPa}$
3.3.5 Effect of inter-particle friction coefficient ($\mu$)

Effect of inter-particle friction coefficient representing surface roughness has been investigated using PFi simulation series. A series of penetration tests have been performed on loose ($D_{rc}=25\%$) and very dense ($D_{rc}=85\%$) assemblies with particle frictions of 0.05, 0.2, 0.4, 0.5, 0.6 and 0.7. As illustrated in Figure 3-34a and Figure 3-34b, $q_{cN}$ and $f_{sN}$ increase as the inter-particle friction increases. A similar trend has been reported by (Falagush et al. (2015b), Khosravi et al. (2019)) regarding an increase in penetration with inter-particle friction coefficient using DEM. The variations of $q_{cN}$ on normalized vertical effective stress show that after $\mu=0.5$, the change in tip resistance is less affected by the increase in particle friction. This is confirmed in Figure 3-34d where the slope of $D_{rc}$-$q_{cN}$ is majorly influenced by the change of $\mu$ from 0.05 to 0.5 with insignificant variation observed in higher $\mu$ values. At lower values of $\mu$, the translations of particles is dominated by the sliding mechanism, where at higher values of $\mu$ these translations are predominantly dominated by the rolling mechanism (Thornton (2000), Kruyt and Rothenburg (2006)). Concerning the SBT classification, it is observed in Figure 3-34e that increasing the particle friction shifts the data towards the top and top left side of the chart in very dense and loose assemblies, respectively. These observations are consistent with that of the calibration procedure, where higher values of $\mu$ lead to a more dilative response in granular assembly (Belheine et al. (2009)).

Figure 3-35 illustrates the variations of small-strain shear wave velocities on normalized effective vertical stress and the variation of shear wave velocities at 100 kPa vertical pressure for assemblies with various inter-particle friction coefficients. The friction is changed after consolidation and $S$-wave is generated through the bedrock to be received via RVEs. As can be seen, $V_s$ increases with increasing $\mu$ for both loose and very dense assemblies. However, this effect dissipates at $D_{rc}=85\%$ for the different values of $\mu$. A significant jump is observed in $V_s$ for the shift between $\mu=0.2$ to 0.4, while after $\mu=0.5$, the shear wave velocities are quite similar. It is interesting to note that assemblies with no friction present a very low $V_s$ in different confinement stresses. It can be concluded that higher surface roughness in particles leads to higher shear wave velocities in granular assemblies.
As discussed above, the translations of the particles are predominantly dominated by the sliding mechanism at lower values of inter-particle friction. This can be observed in the distribution of the particle displacements for assemblies with various \( \mu \) values in Figure 3-36 and Figure 3-37. Considering the force chain distributions, changes in \( \mu \), affect the interactions between the probe and particles as no strong normal force is mobilized for assemblies with \( \mu \) less than 0.2. The strong contact forces are mobilized and increased with the values of \( \mu \) above 0.4, with higher magnitudes and sparser distributions in the very dense assemblies. This agrees with the CPT measurements obtained from assemblies with various inter-particle frictions (Figure 3-34).
Figure 3-34: variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) normalized $q_c$ in terms of normalized vertical pressure, d) $q_{c1N}$ in terms of $f_{s1N}$ and e) SBT chart of the assemblies with different interparticle friction coefficient ($\mu$)
Figure 3-35: Shear wave velocity measurements for loose and very dense packings with different inter-particle friction ($\mu$)
Figure 3-36: Distribution of particle displacements at the end of penetration in loose assemblies with different inter-particle friction coefficients: (a) $\mu=0.05$, (b) $\mu=0.2$, (c) $\mu=0.4$, (d) $\mu=0.5$, (e) $\mu=0.6$ and (f) $\mu=0.7$
Figure 3-37: Distribution of particle displacements at the end of penetration in very dense assemblies with different inter-particle friction coefficients: (a) $\mu=0.05$, (b) $\mu=0.2$, (c) $\mu=0.4$, (d) $\mu=0.5$, (e) $\mu=0.6$ and (f) $\mu=0.7$
Figure 3-38: Strong contact force chain map distribution at the end of penetration in loose assemblies with different inter-particle friction coefficients: (a) \( \mu = 0.05 \), (b) \( \mu = 0.2 \), (c) \( \mu = 0.4 \), (d) \( \mu = 0.5 \), (e) \( \mu = 0.6 \) and (f) \( \mu = 0.7 \)
Figure 3-39: Strong contact force chain map distribution at the end of penetration in very dense assemblies with different inter-particle friction coefficients: (a) $\mu=0.05$, (b) $\mu=0.2$, (c) $\mu=0.4$, (d) $\mu=0.5$, (e) $\mu=0.6$ and (f) $\mu=0.7$
3.3.6 Effect of particle shape (A.R and $\eta$)

Grain shape has been recognized as a factor affecting the stress-strain relationships and failure criteria of granular deposits (Deresiewicz (1958)). The excessive rotation of disks and spheres in DEM is an assumption that does not reflect the reality occurring at microscale in granular assemblies. Modeling actual particle shapes is an arduous task as intricate imaging techniques are required to capture the particle angularity and shape. Therefore, two alternative approaches are commonly used within practitioners to capture particle angularity and shape in DEM simulations. Clump theory embedded in PFC (Itasca Consulting Group Inc. (2016)) can be used to simulate particles with different aspect ratios. These particles are generated using pebbles that are rigid in local contacts and shape together to model a global particle with specific inertia and volume. Using number of pebbles increases the contacts and coordination numbers (CN) within a packed assembly, resulting in increased computational effort in DEM simulations. Another approach in modeling particle shape is to model the torque generated from the angularity using a rolling resistance stiffness at contacts (e.g, Iwashita and Oda (1998a), (1998c), Shodja and Nezami (2003), Mohamed and Gutierrez (2010), Jiang et al. (2015b), Zhou et al. (2017)). This perfectly plastic model uses rolling resistance coefficient ($\eta$) as a limit for the initiation of plastic deformations within local contacts. Despite the helpful simplification in this approach, the effect of fabric is neglected since rolling stiffness is applied in all directions. In this study, both approaches have been adopted to compare between the CPT measurements and obtain a good insight into representative particle shape effects within DEM. Figure 3-40a shows the scanning electron microscopic (SEM) images of Fraser river sand captured by Jones (2017). The particles of the calibrated sand are angular to sub-angular; accordingly, three clumps with aspect ratios of 1, 1.5 and 2 were chosen for the A.Ri DEM simulations (Figure 3-40b). As for RRi simulations, $\eta = 0.0, 0.2, 0.3$ and $0.4$ were used as rolling resistance coefficients applied in between contacts. Two tests with inhibited rolling were performed to compare the results between the different constitutive models.

Figure 3-41a and Figure 3-41b illustrates the variations of $q_{\text{CN}}$ and $f_{\text{CN}}$ for loose and very dense assemblies generated using the mentioned approaches. It is observed that both $q_{\text{c}}$
and $f_s$ are strongly affected by the particle shape and angularity. This is due to the increased interlocking and rolling resistance between the particles (Falagush et al. (2015a)). A jump in the tip and sleeve resistance is observed for a change of $\eta$ from 0.0 (free rolling) to 0.2 and A.R=1 (single sphere) to A.R to 1.5. However, the difference in CPT measurements becomes less significant for the change of A.R=1.5 to A.R=2 and accordingly $\eta=0.4$ to inhibited rolling. This means that the values of $\eta$ used between 0.1 to 0.4 can successfully impede the excessive rotation of the particles and capture the true nature of sand grains. According to Figure 3-41c, for both approaches, $q_{cN}$ increases with increasing normalized vertical stress. This trend is amplified for higher values of $\eta$ and A.R. The slope of $D_{rc}$-$q_{cN}$ is majorly influenced by the change of $\eta$ from 0.0 to 0.2, with similar shift observed in the change of A.R=1 to A.R=1.5. Although no actual correlation between rolling resistance values and clump shapes exists, the results of simulations containing particles with A.R=1.5 compare favorably with the baseline calibrated simulations ($\eta=0.4$); therefore, A.R=1.5 can be a good representative of the whole physical sample angularity. In terms of SBT classifications, it is observed in Figure 3-41e for both approaches that a shift occurs towards the top left side of the graph as rolling resistance or particle aspect ratio increases, from a transitional contractive and sand with contractive behavior to sand with dilative behavior.

![Sample SEM image of Fraser river sand](image)

![Particle shapes simulated using DEM clump theory](image)

**Figure 3-40:** a) Sample SEM image of Fraser river sand b) particle shapes simulated using DEM clump theory
Figure 3-42 and Figure 3-35 illustrate the variations of small-strain shear wave velocities on normalized effective vertical stress and the variation of shear wave velocity at 100 kPa vertical pressure for assemblies with various rolling resistance friction coefficients and particle shapes (A.R). The rolling resistance is changed after consolidation and S-wave is generated through the bedrock to be received via RVEs. As can be seen, $V_s$ increases with increasing $\eta$ for both loose and very dense assemblies. A significant shift is observed for the assemblies with no rolling resistance. Similar trend is observed for assemblies with aspect ratio of 1. However, marginal difference is observed when the values of $\eta$ and A.R go above 0.3 and 1.5, respectively. It is worthy to note that inhibited rolling culminates in similar values of shear wave velocities compared to the regular $\eta$ approach. All details considered, it can be concluded that particle shape and angularity highly affect the shear wave velocity in granular assemblies.

Figure 3-43 and Figure 3-44 illustrate the distribution of particle displacements at the end of penetration for assemblies with different values of $\eta$. As can be seen, the extent of the zone with high particle displacements, as well as the magnitudes of the particle displacements, decrease with increasing rolling resistance from 0 to 0.2. However, no significant difference is observed for values of $\eta$ above 0.3. The distributions of the strong contact forces in assemblies with different rolling resistance values are presented in Figure 3-45 and Figure 3-46. The contact forces with magnitudes less than 100 N are eliminated for better illustration. The effect of particle shape is evident as larger contact forces are mobilized around the probe in loose assemblies with increasing rolling resistance from 0 to 0.2. For values above $\eta=0.3$, no significant difference is observed in force chain distributions. This is in accordance with the effect of rolling resistance on $q_c$ values presented in Figure 3-41. In very dense assemblies, similar trend is observed with sparser contact distributions around the cone and the frictional sleeve.
Figure 3-41: comparison of the variations of a) $q_cN$ on relative penetration, b) $f_N$ on relative penetration, c) $q_cN$ in terms of normalized vertical pressure, d) $q_cN$ in terms of $D_{rc}$ and e) SBT chart of the assemblies with different rolling resistance coefficient ($\eta$) and aspect ratios (A.R)

(a) (b) (c) (d) (e)

Figure 3-42: Shear wave velocity measurements for the effects of rolling resistance coefficient ($\eta$) and particle shape (A.R) in loose and very dense assemblies
Figure 3-43: Distribution of particle displacements at the end of penetration in loose assemblies with different rolling resistance coefficients: (a) \( \eta = 0 \), (b) \( \eta = 0.2 \), (c) \( \eta = 0.3 \), (d) \( \eta = 0.4 \) and (e) inhibited rolling
Figure 3-44: Distribution of particle displacements at the end of penetration in very dense assemblies with different rolling resistance coefficients: (a) $\eta=0$, (b) $\eta=0.2$, (c) $\eta=0.3$, (d) $\eta=0.4$ and (e) inhibited rolling
Figure 3-45: Strong contact force chain map distribution at the end of penetration in loose assemblies with different rolling resistance coefficients: (a) $\eta=0$, (b) $\eta=0.2$, (c) $\eta=0.3$, (d) $\eta=0.4$ and (e) inhibited rolling.
Figure 3-46: Strong contact force chain map distribution at the end of penetration in very dense assemblies with different rolling resistance coefficients: (a) $\eta=0$, (b) $\eta=0.2$, (c) $\eta=0.3$, (d) $\eta=0.4$ and (e) inhibited rolling.
3.3.7 Effect of cone angle

CA\(\theta^\circ\) simulation series were performed to investigate the effect of different cone angles (\(\theta^\circ\)) with the same diameter on CPT measurements and soil behavior. Johnson (2003) theoretically studied the effect of cone angle on tip resistance, explaining that cone tip should start at a relatively high value for cone angles below 15°, and initially decreases to a minimum value and then increases again as \(\theta^\circ\) increases. These claims were confirmed experimentally through the observations of Gill (1968), Nowatzki and Karafiath (1972).

Here, a series of simulations were performed on loose and very dense sand using probes with cone angles of 45°, 60°, 90° and 120° degrees. Figure 3-47a illustrates the variations of \(q_{cN}\) throughout the penetration. The tip resistance increases significantly with increasing cone angle. Similar observations were obtained by Lin and Wu (2012), using DEM to model miniature CPT with various cone angles. This is due to the lower contact area generated in higher cone angle geometries and increased contribution of elastic deformation of microstructural elements (Johnson (2003)). According to Figure 3-47b, the influence of cone angle on sleeve friction has been negligible. This is predictable as the diameter of the probe and the effective sleeve frictional area does not change in these test series.

The effect of normalized vertical stress on \(q_{cN}\) is presented in Figure 3-47c. As can be seen, increasing the mean effective stress increases the elastic response of the assembly to the cone and tip resistance increases consequently. As for the SBT classification in Figure 3-47d, since the sleeve friction is not influenced significantly, the soil behavior does not alter from a dilative response, with an inclination towards the upper left side of the plot.

Figure 3-48 and Figure 3-49 illustrate the distribution of particle displacements at the end of penetration for loose and very dense assemblies with different cone angles. As can be seen, the extent of the zone with large particle displacements increase with increasing the cone angle in assemblies. particles with high displacements as much as 10 cm are generated around the cone in probes with cone angle of 90° and 120°. Figure 3-50 and Figure 3-51 illustrate the distribution of the strong contact force map distributions at the end of penetration for loose and very dense assemblies with different cone angles. The contact forces with magnitudes less than 100 N are eliminated for better illustration.
Stronger contact forces are generated near the tip of the probe in cones with higher cone angles in both loose and very dense assemblies. This agrees with higher $q_c$ values observed in these probe configurations (Figure 3-47).

Figure 3-47: variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) normalized $q_c$ in terms of normalized vertical pressure, d) $q_{c1N}$ in terms of $f_{s1N}$ and e) SBT chart of the assemblies with different cone angles
Figure 3-48: Distribution of particle displacements at the end of penetration in loose assemblies with different cone angles: (a) 45°, (b) 60°, (c) 90° and (d) 120°
Figure 3-49: Distribution of particle displacements at the end of penetration in very dense assemblies with different cone angles: (a) 45°, (b) 60°, (c) 90° and (d) 120°
Figure 3-50: Strong contact force chain map distribution at the end of penetration in loose assemblies with different cone angles: (a) 45°, (b) 60°, (c) 90° and (d) 120°
Figure 3-51: Strong contact force chain map distribution at the end of penetration in very dense assemblies with different cone angles: (a) 45°, (b) 60°, (c) 90° and (d) 120°
3.3.8 Compound effect of cone and sleeve friction coefficients

CPT probes erode gradually due to repetitive tests in granular sediments, through which the cone roughens, and frictional sleeve wears over time. This can lead to errors in data interpretation and soil classification estimations. Jiang et al. (2006b), Khosravi et al. (2019) reported an increase in tip resistance for a perfectly rough cone using DEM simulation of CPT. Jekel (1988), DeJong and Frost (2002) have reported the importance of sleeve surface roughness on $f_s$. Therefore, the combined effect of probe-particle interface friction has been investigated in this study using PFi simulation series. Figure 3-52a and Figure 3-52b demonstrate the variations of $q_{cN}$ and $f_{sN}$ for different cone and sleeve
Figure 3-52: Variation of a) $q_{cN}$ in terms of relative penetration, b) $f_{sN}$ in terms of relative penetration, c) $q_{cN}$ in terms of normalized vertical pressure, d) $q_{c1N}$ in terms of $f_{s1N}$ and e) SBT chart of the assemblies considering probe wear

interface friction coefficients. For the sake of brevity, the results of penetration simulations on loose ($D_{rc}=25\%$) have been presented. The results of the total smooth cone and sleeve are illustrated in Figure 3-52c and Figure 3-52d for comparison. Merely 36% increase is observed for cone friction change from 0.0 to 0.5, while $f_{sN}$ significantly increases with sleeve friction coefficient. It is clear that sliding is the dominating interface failure mechanism in a frictional sleeve and $f_{s}$ significantly depends on the value
of sleeve friction coefficient, while the tip resistance is primarily dominated by the elastic deformation of the microstructural elements (Johnson (2003)). It is observed in Figure 3-52e and Figure 3-52f that the effect of probe friction coefficient on \( q_{cN} \) is more pronounced at higher relative densities. In terms of SBT classification, a shift towards the right side of the chart (TD) is observed as the probe wears over time (Figure 3-52g).
3.4 Discussion on the effect of microparameters on soil behavior and CPT measurements

As discussed in previous sections, various studies have shown that the change in the microparameters such as modulus, inter-particle friction coefficient, rolling resistance coefficient, probe frictional properties, or macro-parameters such as probe geometry and particle aspect ratio are influential on shear strength and behavior of granular materials. Therefore, it is beneficial to outline the effect of these parameters in terms of soil classification and behavior for penetration problems. The effect of the different parameters on variations of SBT classification has been plotted in Figure 3-53 (Robertson (2016)). An upward shift towards a more dilative response is observed with decreasing void ratio of the assemblies, consistent with higher mean effective stress generated around the cone. An upward shift is also observed for the increase in $\mu$, $\eta$ and A.R. However, increasing particle surface roughness ($\mu$) primarily affects the dilation angle of the assembly while particle shape ($\eta$ or A.R) increase shear strength of the assembly. Particle compressibility ($E^*$) has shown a negligible effect on the behavior of the material according to DEM results. Admittedly, cone angle and cone erosion generate an inclination towards the left and right side of the SBT charts, respectively.

Micro parameters such as grain angularity, grain shape, surface roughness, or other factors discussed in this study were not considered in the development of the SBT charts. However, knowledge of the effect of these parameters on soil behavior and classification facilitates the interpretation of field penetration test results and leads to more accurate design in geotechnical problems.
3.5 Conclusion

3D DEM simulations of cone penetration tests were provided in this study to investigate the effect of microparameters, probe geometry, and state on $q_c$ and $f_s$ measurements. Assemblies of spheres were modeled using a high gravitational field with periodic boundaries to mimic the field test conditions. The results of the DEM simulations presented a satisfactory agreement with those observed using miniature calibration chambers test on FRS. The obtained profiles of $q_{cN}$ and $f_{sN}$ increase continuously throughout penetration similar to the observations in centrifuge modeling. Due to higher mean effective stress, $q_c$ and $f_s$ measurements increase with increasing vertical stress and $D_{rc}$.

It was observed that changes in particle compressibility does not affect the CPT measurements significantly. Contrarily, increasing particle angularity (rolling resistance coefficient and particle aspect ratio) and particle friction coefficient increases the $q_c$ and
fs measurements. Further comparison showed that particles with A.R=1.5 represent the behavior of the calibrated sand perfectly. Investigation on the probe properties showed that increasing cone angle increases qc but has negligible effect on fs measurements. This is due to the higher contact area and the resulted elastic deformation of the microstructural elements. Concerning the probe wearing, it was observed that both cone and sleeve friction increase with increasing cone friction coefficient. However, a low choice of friction coefficient is not recommended for the frictional sleeve as fs is dominated by the interface frictional failure mechanism.

Respecting the SBT classification, increasing particle angularity, friction and Drc shift the behavior of soil from a contractive to a more dilative response. Particle compressibility (E*) was found to have negligible effect on soil behavior. Increasing cone angle and probe wear moved the data towards the left and right side of the chart, respectively. Comprehensive knowledge of the microparameters on CPT measurements illuminates the real behavior of granular soils and presents a unique contribution to a more sophisticated and accurate design.
Chapter 4

4 Instability of Granular Materials Under Simple Shear Failure Mode: A DEM Perspective

Within the confines of this chapter, Discrete Element Method (DEM) has been used to study the instability of granular materials under drained and undrained failure conditions. 3D assemblies of the stacked-ring simple shear device were modeled to simulate monotonic constant volume, constant stress, and drained constant shear stress paths. Using the critical state framework, the trends of undrained yield strength ratios on state parameter were proposed.

4.1 Introduction

The inability of a soil medium to sustain the applied external load is called Instability (Skopek et al. (1994), Chu et al. (2003)). Static liquefaction is a form of instability that occurs in loose sands due to pore water pressure generation that is triggered by the undrained shear loading prior to failure (Sadrekarimi (2020)). Another form of instability that occurs in fully drained condition is triggered by the reduction in mean principal effective stress associated with an increase in pore pressure, while the shear stress remains constant (Skopek et al. (1994), Chu et al. (2003), Daouadji et al. (2010), Dong et al. (2016)). Since no peak is observed in the stress path of this type of failure, the prediction of instability in the drained failure of slopes is an arduous task in the practice. Therefore, it is important to understand the concepts of drained and undrained instabilities in geotechnical design and analysis to prevent the following catastrophic repercussions.

Several studies have used Direct Simple Shear test to study the instability and liquefaction potential of saturated sands and tailings. Direct Simple Shear (DSS) test has gained popularity among practitioners due to its simplicity and capability to capture the in-situ conditions applied to the soil such as plane-strain shearing and $k_0$ consolidation. Stacked-ring device developed by (Ishihara and Yamazaki (1980)) has been proven to replicate the rotation of the shearing plane in an excellent fashion. The specimen is
covered with a latex membrane, confined within a set of frictionless steel rings. The rings allow for shearing movements along multidirectional loads. However, incomplete measurements of stress components and neglecting the principal stress rotations in the laboratory have culminated in challenges in interpreting the results obtained from this test. Through a series of monotonic DSS tests on sand, Budhu (1979) found out that deformation occurs uniformly only in the mid-one-third section of the sample, and stress localization is observed in the boundaries. Furthermore, lack of instrumentation in this device impedes the measurement of intermediate principal stress ($\sigma'_{2}$) as an important factor in defining the shearing behavior of soil. In this regard, researchers have used numerical methods to overcome these complexities.

Many attempts have been performed to simulate simple shear test using continuum methods (Budhu and Britto (1987), Dounias and Potts (1993)). In general, inhomogeneous stress distribution along the DSS sample was observed using both modified Cam-Clay and isotropic Elasto-Plastic models. Despite the convenience of the mentioned constitutive models, they are incapable of modeling the principal stress-strain rotation. Therefore, complex constitutive models that account for the rotation of principal stresses such as the combined plastic potential and double shear theory (Yu and Yuan (2006)), the hypoplasticity theory (Tejchman and Bauer (2005)), and the yield vertex theory (Yang and Yu (2006)) have been used to simulate simple shearing. In excess of these challenges, the discrete nature of the granular soils contradicts the assumption of continuity used in the Finite Element Method (FEM).

Developed by Cundall and Strack (1979), Discrete Element Method (DEM) has gained approval among geotechnical engineers due to its ability to replicate the distinct nature of granular materials and more importantly the large deformation failures. The first attempt to capture DEM-based simple shearing behavior of granular materials was carried out by Matsuoka et al. (1988). Through simulation of Cambridge DSS test in a plane-strain condition, they observed a rotation of principal stresses of about 33° to 35° at the peak stress ($\gamma = 5\%$). Katagiri et al. (2010) tried to simulate constant stress and constant volume behavior of particles with irregular shapes. 3D-DEM assemblies of clumps with 4 and 10 elements were modeled based on X-Ray CT images of sand particles. The
boundaries were chosen as periodic to reduce the inhomogeneities. Using inter-particle friction angle varying between $0^\circ$ and $27^\circ$, dense and loose assemblies were obtained in consolidation. As observed, 10 element clumps showed better agreements with the actual shear strength of the sand. However, in the constant volume tests, assemblies reached static liquefaction at a lower void ratio compared to the experiments, marking the necessity to use more complex particle shapes. Dabeet, A., Wijewickreme, D., Byrne (2011) simulated simple shearing using DEM and calibrated the nonlinear model parameters with assemblies of glass beads. 10000 particles were generated within the boundaries and their radii expanded until the model state was reached. The friction coefficient between the upper and lower walls was chosen as high as 10 to minimize the particle sliding adjacent to the plates. As observed, the force chains were parallel with the vertical stress after consolidation. At 4% shearing, the strong force chains rotated significantly due to rotations of principal stresses, to align with the direction of maximum principal stress ($\sigma'_1$). In the same vein, Dabeet et al. (2015) evaluated the stress-strain nonuniformities occurring within a DSS sample. They stated that reading the stresses from the boundaries leads to an overestimation due to nonuniformities along the borders. Despite the thorough research performed on the simple shearing behavior of materials, very few researches have been carried out to investigate the instability, static liquefaction and critical state behavior of granular materials in a micromechanical medium.

Within the confines of this study, drained and undrained instability of granular assemblies are investigated under simple shear stress path. Several studies have reported the ability of DEM to capture the critical state behavior of granular materials in drained and undrained stress paths (Sitharam et al. (2007), Huang (2014), HUANG et al. (2014), Barnett et al. (2019), Ciantia et al. (2019), Rahman et al. (2021)). Therefore, the results are described within the framework of critical state soil mechanics to assess the static liquefaction susceptibility of DEM assemblies.
4.2 Discrete Element Method (DEM)

Particle Flow Code (PFC3D.6) from Itasca has been used to simulate the DSS tests and calibrate the microparameters in a DEM-based platform. It is evident that the quasi-static behavior of granular assemblies is highly sensitive to the particle shape irregularities (Holtz and Kovacs (1981), Shinohara et al. (2000), Terzaghi and Peck (2010), Altuhafi et al. (2016)). Various studies (Iwashita and Oda (1998b), (2000), Mohamed and Gutierrez (2010), Wensrich and Katterfeld (2012), Zhou et al. (2017)) have used a rolling resistance coefficient between contacts to mimic the moment acting between angular particles. For this reason, Rolling resistance linear model embedded in PFC3D.6 (Itasca Consulting Group Inc. (2016)) has been used to simulate DSS samples. In this formulation, a contact moment ($\vec{M}_r$) is defined alongside the local normal ($\vec{F}_n$) and shear ($\vec{F}_s$) forces. The increments of these parameters in a DEM cycle are calculated as below:

\[
\Delta \vec{F}_n = K_n \Delta \vec{U}_n \\
\Delta \vec{F}_s = K_s \Delta \vec{U}_s \\
\Delta \vec{M}_r = K_r \Delta \vec{\omega}_r
\]

[Eq. 1]

Where $\Delta \vec{F}_n$, $\Delta \vec{F}_s$, and $\Delta \vec{M}_r$ are the increments of local normal force, shear force and moment applied in contacts, $K_n$, $K_s$, and $K_r$ are the normal, shear and rolling resistance stiffnesses, and $\Delta \vec{U}_n$, $\Delta \vec{U}_s$ and $\Delta \vec{\omega}_r$ are the increments of relative normal displacement, shear displacement and rotation at the contact positions, respectively. Details of the model used can be found in Ai et al. (2011). The deformability method incorporated in PFC uses a soft contact approach, through which the deformability of a DEM assembly is fit by an isotropic material model. Accordingly, the normal, shear and rolling resistances can be related to the effective modulus ($E^*$) and normal-to-shear stiffness ratio ($k_{ratio}$) as below:

\[
K_n = E^* A/L \\
K_s = K_n/k_{ratio}
\]

[Eq. 2]
\[ K_r = K_s R_A R_B \]

In which \( A \) is the contact area \( (A=\pi r^2) \), \( L \) is the distance between the contacting particles, \( R_A \) and \( R_B \) are the radii of two touching particles. Linear elastic model in normal direction and elastic-perfect plastic model are attributed to the contacts for shear force and moment calculations. Accordingly, sliding and rolling merely occur if the following conditions satisfy during a DEM cycle:

\[ \| \vec{F}_s \| \geq \mu \| \vec{F}_n \| \]

\[ \| \vec{F}_s \| \geq \eta \frac{R_A + R_B}{2} \]  

[Eq. 3]

Where \( \mu \) and \( \eta \) are the friction and rolling resistance coefficients.

### 4.3 DEM modeling methodology

#### 4.3.1 Calibration of microparameters

As demonstrated, five micromechanical parameters including Particle density \((\rho)\), Effective modulus \((E^*)\), Normal to shear contact stiffness \((k_\text{ratio})\), Inter-particle friction coefficient \((\mu)\) and Inter-particle rolling resistance coefficient \((\eta)\) have to be calibrated to capture the behavior of sand. For this reason, a series of Drained Triaxial Tests (DTT)s and odometer tests were performed and compared to best fit the macro-response of Fraser river sand (Karimian (2006), Ghafghazi et al. (2014), Jones (2017)) as a uniform compressible granular material to calibrate the micro-parameters. Figure 4-1 demonstrates the particle size distribution (PSD) curve of the Fraser river sand (FRS) and the adopted assemblies for DSS simulation in this study. The minimum and maximum void ratios of the sand are 0.63 and 0.96, respectively. The DEM Triaxial specimen is a cylinder with an approximate height to diameter ratio of 2 (7 mm wide and 15 mm high), comprising 10000 spheres with a similar gradation of the baseline sand (Figure 4-2b). The particles were generated within the boundaries of the specimen in a cloud of overlapping particles; afterward, cycles were performed to minimize their overlap. In this stage, the sample was compressed to the required confining pressures using the
servomechanism applied to the top and bottom rigid walls. The servomechanism applied to the radial boundary allowed the walls to change in diameter to maintain a constant confining pressure (25 kPa and 35 kPa). During this step, the interparticle friction coefficient was chosen as low as 0.05 to obtain a dense sample with a void ratio of 0.69 corresponding to the experimental observations. After the compaction, the deviatoric load is applied by the top wall at a constant rate. Obtaining the calibrated microparameters, DTT at higher confining pressure (100 kPa) was simulated as well to guarantee the volumetric behavior.

The simulation of the odometer test is to confirm the validity of the parameters obtained in the calibration procedure (Figure 4-2a). The odometer sample consists of a rigid cylinder confined with two walls on top and bottom. The assemblies are made with 5000 spheres with gradation similar to that of FRS. The sample packing procedure is similar to the DTT; however, the inter-particle friction coefficient has been chosen at a high value of 0.5 to obtain loose specimens corresponding to the experimental test conditions. The samples are compacted to 10 kPa and then loaded vertically using stress-controlled top wall to the desired stresses while the radial wall facets remain unchanged (1D compression test). The void ratio variation of the sample is read using the measurement spheres embedded at the center of the sample.
Figure 4-1: PSD curve of Fraser river sand and the adopted assemblies
Confirmed observations of some sensitivity analyses performed by (Belheine et al. (2009), Hazeghian and Soroush (2015), Coetzee (2017)), help calibrate the microparameters. As suggested:

- The Poisson’s ratio ($k_{ratio}$ in micromechanics) of the material is related to the initial slope of the volumetric strain diagram.
- The initial slope of the stress-strain diagram is related to the effective modulus ($E^*$) of the material

Figure 4-2: Samples of a) Odometer test and b) Triaxial test simulated for calibration of micro-parameters
• η and μ both significantly affect the stress-strain curve by increasing the peak and residual strengths of the material. To overcome this cross dependency, it should be noted that η has a negligible effect on the dilatancy curve. Therefore, a series of tests are performed to fit the dilatancy curve and obtain the corresponding dilatancy angle (ψ) of the material by varying μ. Afterward, η is changed to fit the stress-strain curve of the material with the experimental results, to obtain the corresponding peak and residual friction angles.

Table 4-1 presents the calibrated microparameters used in this study.

Table 4-1: Calibrated micromechanical parameters used in this study

<table>
<thead>
<tr>
<th>Micro material parameters</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle density (kg/m³), ρ</td>
<td>2690</td>
</tr>
<tr>
<td>Modulus of elasticity of contact (MPa), E</td>
<td>100</td>
</tr>
<tr>
<td>Normal to shear contact stiffness, ( k_{ratio} )</td>
<td>1.5</td>
</tr>
<tr>
<td>Inter-particle friction, ( \mu )</td>
<td>0.7</td>
</tr>
<tr>
<td>Inter-particle rolling coefficient, ( \eta )</td>
<td>0.4</td>
</tr>
<tr>
<td>Non-local damping coefficient, ( \alpha )</td>
<td>0.1</td>
</tr>
</tbody>
</table>

4.3.2 Methodology to simulate DEM-DSS

It is aimed to simulate the DSS stacked ring device using DEM in the present study (Figure 4-4a). The cylindrical assembly is peripherally confined with 10 rings and two plates on top and bottom. The rings have a diameter of 70 mm and are 2-mm-thick, achieving a sample with a final 20-mm height. As indicated by (Shen et al. (1978), Amer et al. (1987)), the stress distribution inside the sample is more uniform when the ratio of
the height to the diameter of the specimen ($H/D$) decreases. DEM-based observations of Chang et al. (2016) indicate that $H/D$ values ranging between 0.2 to 0.4 produce a uniform force chain distribution in the core zone of the model, confirming the validity of the ratio used in this study ($H/D=0.28$).

The particle assembly is generated within the domain of the test as a packed assembly with huge overlaps. DEM cycles are performed to minimize the overlaps and maintain balance within the system. Then, the sample is consolidated using the stress-controlled top platen. At this stage, a high value of $\mu = 1$ was chosen in conjunction with rolling resistance to increase the interlock between the particles and obtain an assembly in its loosest state. This parameter was set back to its initial calibrated value after the consolidation stage. Additional cycles are applied to the model to minimize the unbalanced forces and maintain equilibrium before shearing. Shearing is applied by giving a strain rate to the bottom plate and the rings in the horizontal direction. The particles adjacent to the platens are forced to move with the plates to apply the shear stress to the assembly in a uniform manner and replicate the roughness of the porous stones.

Frictional boundaries in DSS could produce complementary shear stresses at the specimen boundaries and help equalize the specimen. As suggested by Bernhardt et al. (2016), the interface friction angle between the rings and the particles was chosen as 19.8°, representing the friction between latex membrane and spheres in experiments. To investigate the effect of side boundary, three drained simulations with fewer particles on loose sand are performed with different boundary friction coefficients of 0.0, 0.36 and 0.5. The variations of shear stress and volumetric strain with the development of shear strain for specimen with different boundary friction coefficients are presented in Figure 4-3. A softer response is observed for simulation with frictionless boundary condition. Dabeet et al. (2015) observed a stress ratio difference of 0.06 at 4% shear strain for two conditions; however, they did not report the effect of lateral boundary condition on volumetric behavior of the assembly.
The strain rate for constant volume and constant stress samples varies linearly within the rings between 0.1mm/s for the bottom plate and the ring adjacent to it to zero for the top plate and the ring adjacent to it (Figure 4-4b). This method provides a uniform shear strain along with the depth of the sample (Asadzadeh and Sorouch (2016)). The timestep in the simulations was chosen as $10^{-6}$ considering the Railey’s wave and the critical timestep. Shear stress is computed using the average stress tensor ($\bar{\sigma}_{ij}$) in the entire vessel volume ($V$):

$$\bar{\sigma} = -\frac{1}{V} \sum_{N_c} F^{(c)} \otimes L^{(c)} \quad [\text{Eq. 4}]$$

In which $N_c$ is the number of contacts, $F^{(c)}$ is the contact force vector, $L^{(c)}$ is the branch vector connecting the centroids of the contacting particles, and $\otimes$ is the outer product notation. Using this approach, the values of the horizontal component in stress tensor can be obtained after the consolidation. Figure 4-7 illustrates the variations of $k_0 = \sigma'_{xx}/\sigma'_{zz}$ obtained after consolidation for the simulations of this study. The $k_0$ values range from 0.56 to 0.51, comparing favorably with the method proposed by Jaky. J (1944) for the calculation of the coefficient of earth pressure at rest.
Multiple Representative Volume Elements (RVE)s were embedded into the model domain with different placements to trace the variations of micro and macro parameters in the assembly. As illustrated in Figure 4-5, nine major RVEs named RVE1 to RVE9 are located in xz and yz planes with a radius of 8mm (dashed line circles). 14 Minor RVEs with smaller radii of 4 mm were embedded along the surface of the bottom and top plate to measure the shear stress distribution (solid red line circles).

**Figure 4-4: Schematic of the (a) DEM assembly after consolidation, (b) DEM assembly end of shearing and (c) placement of RVEs in the specimen**
The void ratios measured after consolidation ($\sigma'_{vc}=100$ kPa) using RVE1 to RVE9 are shown in Figure 4-6. As can be seen, the values of void ratios after consolidation ($e_c$) vary between 0.898 to 0.916 for both xz and yz planes in loose assembly. The non-uniformities are primarily generated near the boundaries of the specimen. The non-uniformities reduce with increasing relative density of the sample. Considering the
computational effort, vertical boundary contraction seems a promising method in DEM simulation of a homogeneous DSS sample.

![Graph showing void ratios measured from the RVEs after consolidation (e_c) in xz and yz planes for loose and dense assemblies.

The Index of unbalanced forces (I_{UF}) Ng (2006b) is monitored throughout shearing to control the equilibrium of the assembly. As demonstrated in Figure 4-8, the variations of I_{UF} are maintained below 0.01, a reasonable criterion according to Ng (2006b) to maintain the quasi-static regime within the particle assembly. No gravity is applied during any step of this simulation.

Figure 4-6: Void ratios measured from the RVEs after consolidation (e_c) in xz and yz planes for loose and dense assemblies
Figure 4-7: Coefficients of earth pressure ($k_0$) obtained from the DEM simulations after consolidation

Figure 4-8: Variations of $I_{UF}$ throughout shearing in test with $\sigma'_v=100$ kPa
To obtain the optimum scale size and particle size distribution, various drained DSS tests have been performed with different particle numbers (Figure 4-9). The particle size distributions are shifted proportionally towards the right side of that of FRS using a scaling factor $N$. Bernhardt et al. (2016) through calibration of experimental and DEM samples of DSS tests, observed that the number of particles significantly affects the response of the material and the homogeneity of the specimen. Figure 4-10 demonstrates the stress-strain-volumetric behavior of the specimens generated with different particle numbers. It is observed that the shear strength of the sample is not sensitive to the particle numbers above 5000. The macroscopic stiffness does not change in the simulations as it is proportional to the particle dimensions (Gabrieli et al. (2009)). However, it can be observed that the volumetric behavior is highly sensitive to the particle numbers. A consistent void ratio variation is important as it contributes to the critical state framework used in this study. Regarding these trends, samples with 30000 particles were chosen as the baseline for the simulations in this study. As evidenced by Chang et al. (2016), the nonuniformity of the shear stress is minimized when the ratio of the height of the specimen to the maximum particle size ($H/d_{max}$) is no less than 7 (10 used in this study).

Figure 4-9: Scaled-up specimens for DSS testing corresponding to a) 1053 particles, b) 5300 particles, c) 10380 particles, d) 21405 particles and e) 30000 particles (used in this study)
Table 4-2 summarizes the simulations carried out in this study. A total of 20 simulations including Drained direct simple shear (DCSS), constant volume (CV) simple shear and drained constant shear stress tests are conducted to investigate the instability of granular materials under various stress paths. The drained simple shear tests are performed to complete the critical state line collectively with CV tests. Hereafter, the void ratio after the consolidation is denoted as \( e_c \) and the vertical stress after the consolidation is denoted as \( \sigma'_vc \).

**Figure 4-10:** Variations of a) shear stress on shear strain and b) volumetric strain on shear strain for assemblies with different scaling factors at \( \sigma'_vc = 100 \text{ kPa} \)
<table>
<thead>
<tr>
<th>Test ID</th>
<th>$D_r$ (%)</th>
<th>$e_c$</th>
<th>$\sigma'_{vc}$ (kPa)</th>
<th>$e_{cs}$</th>
<th>$\sigma'_{vcs}$ (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Constant volume</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CV1</td>
<td>20.3</td>
<td>0.893</td>
<td>100</td>
<td>0.893</td>
<td>2.04</td>
</tr>
<tr>
<td>CV2</td>
<td>20.9</td>
<td>0.891</td>
<td>150</td>
<td>0.891</td>
<td>1.62</td>
</tr>
<tr>
<td>CV3</td>
<td>21.5</td>
<td>0.889</td>
<td>200</td>
<td>0.889</td>
<td>1.69</td>
</tr>
<tr>
<td>CV4</td>
<td>24.2</td>
<td>0.880</td>
<td>300</td>
<td>0.880</td>
<td>21.78</td>
</tr>
<tr>
<td>CV5</td>
<td>30.6</td>
<td>0.859</td>
<td>400</td>
<td>0.859</td>
<td>93.82</td>
</tr>
<tr>
<td>CV6</td>
<td>33.3</td>
<td>0.855</td>
<td>450</td>
<td>0.855</td>
<td>119.54</td>
</tr>
<tr>
<td>CV7</td>
<td>35.7</td>
<td>0.842</td>
<td>500</td>
<td>0.842</td>
<td>140.20</td>
</tr>
<tr>
<td>CV8</td>
<td>49.3</td>
<td>0.797</td>
<td>700</td>
<td>0.797</td>
<td>261.60</td>
</tr>
<tr>
<td>CV9</td>
<td>63.6</td>
<td>0.750</td>
<td>1000</td>
<td>0.750</td>
<td>406.39</td>
</tr>
<tr>
<td><strong>Drained</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DR1</td>
<td>20.3</td>
<td>0.893</td>
<td>100</td>
<td>0.818</td>
<td>100</td>
</tr>
<tr>
<td>DR2</td>
<td>20.9</td>
<td>0.891</td>
<td>150</td>
<td>0.820</td>
<td>150</td>
</tr>
<tr>
<td>DR3</td>
<td>21.5</td>
<td>0.889</td>
<td>200</td>
<td>0.814</td>
<td>200</td>
</tr>
<tr>
<td>DR4</td>
<td>22.4</td>
<td>0.886</td>
<td>250</td>
<td>0.819</td>
<td>250</td>
</tr>
<tr>
<td>DR5</td>
<td>24.2</td>
<td>0.880</td>
<td>300</td>
<td>0.811</td>
<td>300</td>
</tr>
<tr>
<td>DR6</td>
<td>30.6</td>
<td>0.859</td>
<td>400</td>
<td>0.796</td>
<td>400</td>
</tr>
<tr>
<td><strong>Drained Constant shear stress</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DCSS1</td>
<td>23.0</td>
<td>0.893</td>
<td>100</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DCSS2</td>
<td>24.0</td>
<td>0.891</td>
<td>150</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DCSS3</td>
<td>24.5</td>
<td>0.879</td>
<td>200</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DCSS4</td>
<td>25.7</td>
<td>0.875</td>
<td>300</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DCSS5</td>
<td>30.0</td>
<td>0.859</td>
<td>400</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
4.4 Results and discussion

4.4.1 Drained simple shear tests

During the drained simulations, a constant vertical stress ($\sigma'_{vc}$) is maintained in shearing through a servo-controlled upper wall. Figure 4-11a and Figure 4-11b demonstrate the stress-strain and volumetric behavior of drained tests. As can be seen, a strain-softening (contractive) behavior is observed in all drained simulations. Figure 4-11b shows that the volumetric behavior of the simulations is asymptotically reaching a steady value (critical state) in the range of applicable strains. An average friction angle at critical state of $\phi'_c=29^\circ$ is obtained in drained tests (Figure 4-11c). The majority of the friction angle is mobilized within the initial 4% of shear strain applied.

In the laboratory setting, the stress state on the vertical plane within a DSS sample is unknown since the principal stresses rotate throughout shearing. For this reason, assumptions are made to obtain the Mohr circle and compute the mobilized friction angle $\phi'_m$. The first method, namely alpha ($\alpha$) method, assumes that the maximum shear stress ($\tau_{xz}'$) occurs at the horizontal plane, in which the mobilized friction angle is:

$$\alpha^\circ = \sin^{-1}\left(\frac{\tau}{\sigma'_{zz}}\right)$$

[Eq. 5]

The other common assumption, namely beta ($\beta$) method, assumes that the horizontal plane is the plane of maximum stress obliquity, in which the mobilized friction angle is:

$$\beta^\circ = \tan^{-1}\left(\frac{\tau}{\sigma'_{zz}}\right)$$

[Eq. 6]

To investigate this discrepancy, the variations of the mobilized friction angle calculated using principal stresses are compared with the mentioned methods. This is possible to capture since DEM uses measurement spheres to compute the variations of stress tensor components (e.g., $\sigma'_{xx}$ and $\sigma'_{zz}$):
\[
\phi_{mob}^o = \sin^{-1}\left(\frac{\sigma_1' - \sigma_3'}{\sigma_1' + \sigma_3'}\right)
\]  
[Eq. 7]

Figure 4-11: Variations of a) Shear stress, b) volumetric strain and c) frictional angle of the DEM specimens in drained simple shear simulations
Figure 4-12a illustrates the mobilized friction angle computed from different methods and DEM on shear strain. As demonstrated, the mobilized friction angle is defined by the \( k_0 \) condition at the initiation of the test (\( \gamma = 0\% \)). Progressively, the mobilized friction angle increases as the shear stress acting on the horizontal plane increases. At the end of the shearing (\( \gamma = 20\% \)), the stress states in the horizontal plane reach the maximum condition and the mobilized friction angle is found to get closer to the \( \beta \) method (Figure 4-12b). The results agree well with the observations of Wijewickreme et al. (2013) obtained from DEM simulation of DSS test. The stress states on the Mohr circle for horizontal and vertical planes are plotted in Figure 4-13 for CV1 and DCSS1 simulations. For both cases, the resultant vertical stress decreases gradually due to generated pore pressure in undrained stress path or unloading in drained constant shear stress path.

Figure 4-12: a) mobilized friction angles obtained from DEM, \( \alpha \) and \( \beta \) method, b) stress states on the Mohr circle for horizontal and vertical planes at the end of shearing
Figure 4-13: stress states on the Mohr circle for horizontal and vertical planes at the end of shearing for a) Constant volume and b) Constant shear stress paths

4.4.1.1 Stress non-uniformity

RVE based interpretation of the results can be challenging since the stress distributions are non-uniform in DSS specimen at larger shear strains. Several studies (Roscoe (1953), Lucks, A. S, Christian (1972), Prevost and Hoeg (1976), Dabeet et al. (2015), Asadzadeh and Soroush (2016)) have reported this inhomogeneity primarily on the lateral boundaries. To quantify this non-uniformity, shear stress and normal stress values were measured using minor RVEs embedded adjacent to the top plate. The placements and size of the RVEs are schematically depicted in Figure 4-5.

Figure 4-14 illustrates the distribution of shear and normal stresses adjacent to the top plate at 20% shear strain from a range of loose to medium dense assemblies. As observed, the variations of both shear and normal stresses are quite uniform in the middle section of the upper boundary, while the non-uniformity exists at the far left and far right RVEs. Measurements of the stresses at the corners of the boundary is not possible since the stresses are basically inter-particle forces divided by a specific area, leading to reduction in stress concentration. For this reason, a quinic polynomial equation with the
form of \( \sigma = f(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 + a_5x^5 \) is used to interpolate and estimate the lateral values. Similar equation has been used by Airey and Wood (1987) to interpolate between the results of the cell pressures. The non-homogeneity of the shear stress and normal stress is clearly observed adjacent to the boundaries. Similar observations were reported by Dabeet et al. (2015), Asadzadeh and Soroush (2016) while evaluating the stress non-uniformities in DSS using DEM. Figure 4-15 illustrates the distribution of shear and normal stresses adjacent to the top plate at three states of consolidation, instability and critical state for CV1 simulation. As can be seen, the stress non-uniformity is the highest at the peak and reduces with increasing shear displacement at the residual state.

![Graph of stress distribution](image_url)
Figure 4-14: Shear and normal stress distributions on the top plate at 20% shear strain for a) $\sigma'_{vc} = 100$ kPa, b) $\sigma'_{vc} = 400$ kPa and c) $\sigma'_{vc} = 700$ kPa
Figure 4-15 Shear and normal stress distributions on the top plate in undrained simulation with $\sigma'_{vc}=100\text{kPa}$: a) after consolidation b) instability c) critical state
4.4.2 Constant volume simple shear tests

To simulate the undrained behavior in DEM, the top plate was secured to maintain the volume constant throughout shearing. In the absence of water, the pore water pressure ($u_w$) that leads to loss of interparticle contacts and the following liquefaction, can be computed as:

$$u_w = \sigma'_{vc} - \sigma'_v$$  \[Eq. 8\]

Where $\sigma'_{vc}$ is the consolidation stress and $\sigma'_v$ is the instantaneous vertical stress. The basic assumption in this approach is that the compressibility of water and soil grains is negligible. CV has been proven as an accurate simplified method to simulate undrained behavior in granular materials (Pickering (1973), Dyvik et al. (1987)).

A series of nine tests with confinements varying between 100kPa to 1000 kPa are simulated in this study. Figure 4-16 illustrates the behavior of the material in CV tests. A strain-hardening behavior is observed in the early stages of all tests (Figure 4-16a). This is in conjunction with a decrease in vertical effective stress and an increase in pore water pressure (Figure 4-16b and Figure 4-16c). This is followed by a strain-softening after reaching a peak value in stress-strain behavior. At this stage, static liquefaction is observed as a form of instability due to the excess pore water pressure. This is clearly observed in steady variations of pore water pressure and vertical effective stress at strain levels about 6%. However, this failure is not observed in tests with high confinements of 700 kPa and 1000 kPa. It should be noted that the initial void ratio of the specimens is not equal after consolidation and the assemblies densify due to consolidation stress.

The stress paths plotted in Figure 4-16d, demonstrate that flow liquefaction has occurred within the granular assembly, as no secondary dilation is observed following the strain softening. Contrary to the CV test results on FRS carried out by (Sivathayalan (1994), Jones (2017)), no phase transformation is observed within the confines of this study in loose materials. This can be attributed to the small surface angularities that are not adequately modeled with rolling resistance (Katagiri et al. (2010)), excluding complex constitutive models that incorporate torsional resistance between particles (Jiang et al.
Admittedly, the absence of fine content in the model assemblies should be considered as it affects the post-liquefaction behavior of granular assemblies. It should be noted that the application of the mentioned solutions is computationally expensive and leads to perplexing simulation complexities.

Figure 4-16: Variations of a) shear stress on shear strain, b) vertical effective stress on shear strain, c) pore water pressure on shear strain and d) stress path and critical state line for CV tests.
A critical state friction angle of $\phi'_{cs} = 28.4^\circ$ is obtained from C.V simulations. The results of the CV simulations can be interpreted in a critical state framework. The critical state is a state in which the soil deforms under constant shear stress, constant pore water pressure and constant void ratio (Casagrande (1936), Schofield and Wroth (1968)). The critical state line (CSL) is the loci of states plotted in the void ratio-logarithm of the effective stress plane as below:

$$e_{cs} = \Gamma - \lambda_{10} log\sigma'_{cs} \quad [\text{Eq. 9}]$$

In which $e_{cs}$ and $\sigma'_{cs}$ are the void ratio and effective vertical stress at critical state respectively; and $\Gamma$ and $\lambda_{10}$ are the line’s intercept at $\sigma'_{cs}=1\text{kPa}$ and slope, respectively. Figure 4-17 depicts the CSL and NCL obtained collectively from DEM and experimental results (Jones (2017)). A linear trend can be perfectly fit with the obtained points as they agree well. Although particle breakage is not considered in this study, a curvature is observed in the CSL in $e$-log $\sigma'_{cs}$ plane. Similar observations were reported by (Ng (2009), Huang (2014)). This indicates that particle breakage is not the only factor that contributes to the curvature in CSL in higher confinement stresses.

Figure 4-17: CSL obtained from DEM and experiments (Jones (2017))
4.4.3 Drained constant-shear-stress tests

Drained constant-shear-stress tests were simulated as a specific stress path that replicates a decrement in confinement stress or an increase in pore water pressure. This type of instability occurs in a fully drained condition in the field under the circumstances of heavy rainfall, increase in the groundwater table, erosion, foundation deformation, etc (Riveros and Sadrekarimi (2020a)).

In these simulations, after consolidation, the assemblies are subjected to an initial shear stress ($\tau_c$). Afterward, a recursive code maintains the shear stress constant with a relaxation factor, permitting no change to the shear stress while the specimen is unloaded vertically at a constant rate. Chu et al. (2011) investigated the effect of the unloading rate and reported a negligible effect on the commencement of instability point. However, faster unloading leads to incomplete pore water pressure dissipation and a decrement in instability stress ratio (Gajo et al. (2000)). Therefore, a low rate of 0.01 kPa/cycle in terms of DEM calculation is chosen for these tests. The stress paths, volumetric behavior and accumulation of shear strain ($\gamma$) are illustrated in Figure 4-18. A dilation followed by continuous contraction is observed after the initial shearing (Figure 4-18b). This behavior corresponds to a gradual increase in shear strain followed by a sharp increase in timestep (Figure 4-18c). Since the assembly never reaches a maximum value in the stress path plane, the definition of the commencement of instability becomes intricate in such failures. The onset of instability in drained failures will be discussed in the following sections thoroughly.
Figure 4-18: a) stress paths, b) volumetric strain, and c) accumulation of shear strain in DCSS simulations

4.5 Evolution of micro parameters

Figure 4-19 and Figure 4-20 demonstrate the evolution of contact force chains in CV and DCSS throughout shearing. The thickness of the force chain lines represents their relative strength. For the CV tests, the contact force networks of the test with \( \sigma'_{vc} = 100\text{kPa} \) are displayed after consolidation, at the onset of instability, and large deformation (critical
state) states. For the DCSS tests, the contact force network of the test with $\sigma'_{vc} = 100$ kPa and $\tau_c = 10.6$ kPa are displayed after consolidation, at the end of initial shearing, and the onset of instability. As observed, both samples have very homogenous contact force distributions after consolidation. Aligned with the maximum principal stress $\sigma'_{vc}$ at the initiation of shearing, the strong contact forces rotate with respect to the vertical axis in both samples, showing the rotation of principal stresses in simple shearing. Note that the reduction in thickness of force chains in DCSS tests is due to the unloading of the vertical stress in this stress path. The buckling of force chains and the generation of localized areas is markedly observed at the onset of instability in both stress paths. With further deformation, the strong force chains align with the maximum principal stress and inhomogeneous stress distribution occurs at the boundaries of the system. Similar observations were reported by (Thornton and Zhang (2006), Asadzadeh and Soroush (2018), Zhang et al. (2019)).

Figure 4-21 illustrates the deformed patterns of the CV1, CV8 and DCSS1 simulations after consolidation and at the end of shearing using a cutting wedge in the middle of the sample. The different attributed colors are only used to clarify the buckling of columns and there will be no influence on the mechanical response of the specimen. Each column comprises of 4 particles in average, stretched along the height of the sample. Similar approach was first used by Jiang et al. (2006a). As can be seen, the particles deform homogenously until the end of shearing in both loose and dense assemblies. No buckling is observed in the columns of colored particles; therefore, it can be concluded that no shear band is initiated in the domains of the samples. This can be attributed to the very low relative density of the sample. Similar observations were reported by Li et al. (2020) when simulating 3D-DEM samples of DSS tests.
Figure 4-19: Evolution of strong contact force distribution a) after consolidation, b) at the onset of instability and c) at critical state in CV1 test
Figure 4-20: Evolution of strong contact force distribution a) after consolidation, b) initiation of constant shear and c) onset of instability in DCSS1 test
Figure 4-21: Particle displacements (a) after consolidation in CV1; (b) at the end of shearing in CV1 (σ'vc=100 kPa); (c) after consolidation in DCSS1; (d) at the end of shearing in DCSS1 (σ'vc=100 kPa); (e) after consolidation in CV8 and (f) at the end of shearing in CV8 (σ'vc=700 kPa)

To further investigate the orientation of the failure plane in DSS specimen, the distribution of the cumulative rotation of the particles is illustrated in Figure 4-22. A cutting wedge is generated in the middle section of the sample to plot the attributed rotation of the particles. The rotation of the particles is normalized to the mean value in DCSS1 and CV1 specimen. As can be seen, the particle rotation distribution is scattered, and no concentrated clear shear band is observed at the sample boundaries. Again, this could be attributed to the low relative density of the sample coupled with a low value of
rolling resistance calibrated for the model. The zone with high gradient of particle rotations is located in the mid-height of the specimen, along with the zero-extension direction of the apparatus. This is in accordance with the trend of the rupture surface proposed by Roscoe (1970).

Figure 4-22: Normalized cumulative particle rotation to the mean value in (a) onset of instability in DCSS1, (b) critical state in CV1 simulation

To quantify the numbers of contacts per particle in a granular assembly, variations of coordination number ($CN$) within the volume of the sample are monitored and presented in Figure 4-23. Starting from the same $CN$ values, this parameter gradually decreases in both CV and DCSS samples, asymptotically reaching a constant value in CV test (critical state). It is worthy to note that the $CN$ values at the onset of instability are similar for both stress paths. A sudden drop is observed in $CN$ variations of DCSS stress path, due to the unloading mechanism occurring in this stress path, leading to fewer possible contacts.
Similar observations were reported by Lashkari et al. (2019) by simulating DEM-based true triaxial specimens, subjected to constant q stress path. The summary of CN values after consolidation, at failure and critical states can be found in Table 4-3 for CV and DCSS simulations performed in this study.

Figure 4-23: Evolution of CN values in CV1 and DCSS1 tests
Table 4-3 Summary of the coordination numbers at consolidation, instability and critical state for CV and DCSS simulations

<table>
<thead>
<tr>
<th>Test ID</th>
<th>$e_c$</th>
<th>$\sigma'_{vc}$ (kPa)</th>
<th>CN (consolidation)</th>
<th>CN (yield)</th>
<th>CN (liq)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Constant volume</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CV1</td>
<td>0.883</td>
<td>100</td>
<td>3.39</td>
<td>3.21</td>
<td>2.65</td>
</tr>
<tr>
<td>CV2</td>
<td>0.881</td>
<td>150</td>
<td>3.46</td>
<td>3.23</td>
<td>2.77</td>
</tr>
<tr>
<td>CV3</td>
<td>0.879</td>
<td>200</td>
<td>3.51</td>
<td>3.26</td>
<td>2.68</td>
</tr>
<tr>
<td>CV4</td>
<td>0.875</td>
<td>300</td>
<td>3.58</td>
<td>3.41</td>
<td>3.04</td>
</tr>
<tr>
<td>CV5</td>
<td>0.859</td>
<td>400</td>
<td>3.77</td>
<td>3.43</td>
<td>3.39</td>
</tr>
<tr>
<td>CV6</td>
<td>0.855</td>
<td>450</td>
<td>3.78</td>
<td>3.48</td>
<td>3.44</td>
</tr>
<tr>
<td>CV7</td>
<td>0.842</td>
<td>500</td>
<td>3.83</td>
<td>3.58</td>
<td>3.50</td>
</tr>
<tr>
<td><strong>Drained Constant shear stress</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DCSS1</td>
<td>0.893</td>
<td>100</td>
<td>3.39</td>
<td>3.20</td>
<td>-</td>
</tr>
<tr>
<td>DCSS2</td>
<td>0.891</td>
<td>150</td>
<td>3.46</td>
<td>3.22</td>
<td>-</td>
</tr>
<tr>
<td>DCSS3</td>
<td>0.879</td>
<td>200</td>
<td>3.51</td>
<td>3.29</td>
<td>-</td>
</tr>
<tr>
<td>DCSS4</td>
<td>0.875</td>
<td>300</td>
<td>3.58</td>
<td>3.35</td>
<td>-</td>
</tr>
<tr>
<td>DCSS5</td>
<td>0.859</td>
<td>400</td>
<td>3.77</td>
<td>3.38</td>
<td>-</td>
</tr>
</tbody>
</table>
4.6 Discussion on the triggering of instability

It is now possible to analyze the triggering of instability in undrained and drained stress paths using the micro and macro parameters. According to Figure 4-16d, instability occurs when the applied shear stress exceeds the $s_u(\text{yield})$, determined from the peak shear stresses in CV tests. Despite the simplicity of this method, it is not applicable in failures with DCSS stress paths in which no peak stress is observed. A more extensive approach suggests the use of “Instability line” (Lade (1992)) passing through the origin and the previously defined point of $s_u(\text{yield})$ in CV stress path plane. Instability occurs when the mobilized friction angle ($\phi'_\text{mob}$) exceeds the slope of the instability line ($\phi'_\text{yield}$).

According to Figure 4-18, the instability in DCSS stress path is brought with a sudden change in shear strain accumulation, while the volumetric strain of the sample varies from dilative to contractive trend. Along with the aforementioned observations, the variations of Second-order work proposed by (Hill (1958)) help define the onset of instability in a granular medium, calculated as:

$$d^2W = \dot{\sigma'}: \dot{\varepsilon} = dev \sigma': dev \varepsilon + p' \dot{\varepsilon}_v$$  \[\text{Eq. 10}\]

In which $\sigma'$ and $\varepsilon'$ are the tensors of the second order of effective stress and total strain, respectively. According to Hill (1958), instability occurs once the abovementioned value becomes negative. Figure 4-24 presents the instability criteria for loose assemblies including instability line, abrupt changes in accumulated shear strain, second-order work, and nullification of volumetric strain in CV and DCSS stress paths for tests with $\sigma'_{vc} = 100, 200 \text{ kPa}$. Despite negligible differences, all the methods are consistent with $\phi'_{\text{yield}}$ obtained in IL method. A similar agreement was achieved by (Chu et al. (2003), Daouadj et al. (2010), Riveros and Sadrekarimi (2020a)) in experimental tests on sand, indicating that static liquefaction is followed by the crossing of IL, with no regards of the stress path applied (Riveros and Sadrekarimi (2020a)).
Table 4-4 Summary of the DSS simulation results

<table>
<thead>
<tr>
<th>Test ID</th>
<th>e&lt;sub&gt;c&lt;/sub&gt;</th>
<th>(\sigma_{ve}') (kPa)</th>
<th>(S_u) (yield) (kPa)</th>
<th>(S_u) (liq) (kPa)</th>
<th>(\phi'_{yield}) (°)</th>
<th>(\phi'_{cs}) (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant volume</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CV1</td>
<td>0.883</td>
<td>100</td>
<td>19.47</td>
<td>2.04</td>
<td>15.04</td>
<td>14.55</td>
</tr>
<tr>
<td>CV2</td>
<td>0.881</td>
<td>150</td>
<td>32.50</td>
<td>1.62</td>
<td>16.87</td>
<td>16.18</td>
</tr>
<tr>
<td>CV3</td>
<td>0.879</td>
<td>200</td>
<td>46.75</td>
<td>1.69</td>
<td>18.54</td>
<td>17.63</td>
</tr>
<tr>
<td>CV4</td>
<td>0.875</td>
<td>300</td>
<td>73.91</td>
<td>21.78</td>
<td>19.91</td>
<td>18.80</td>
</tr>
<tr>
<td>CV5</td>
<td>0.859</td>
<td>400</td>
<td>103.87</td>
<td>93.82</td>
<td>22.51</td>
<td>20.95</td>
</tr>
<tr>
<td>CV6</td>
<td>0.855</td>
<td>450</td>
<td>120.46</td>
<td>119.54</td>
<td>23.04</td>
<td>21.37</td>
</tr>
<tr>
<td>CV7</td>
<td>0.842</td>
<td>500</td>
<td>150.51</td>
<td>140.2</td>
<td>25.76</td>
<td>23.48</td>
</tr>
<tr>
<td>CV8</td>
<td>0.831</td>
<td>700</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CV9</td>
<td>0.811</td>
<td>1000</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Drained</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DR1</td>
<td>0.893</td>
<td>100</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DR2</td>
<td>0.891</td>
<td>150</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DR3</td>
<td>0.889</td>
<td>200</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.886</td>
<td>250</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>-----</td>
<td>------</td>
<td>-------</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>DR4</td>
<td></td>
<td>0.880</td>
<td>300</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DR5</td>
<td></td>
<td>0.859</td>
<td>400</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DR6</td>
<td></td>
<td>0.893</td>
<td>100</td>
<td>-</td>
<td>10.91</td>
<td>14.43</td>
</tr>
<tr>
<td>DCSS1</td>
<td></td>
<td>0.891</td>
<td>150</td>
<td>-</td>
<td>15.58</td>
<td>16.55</td>
</tr>
<tr>
<td>DCSS2</td>
<td></td>
<td>0.879</td>
<td>200</td>
<td>-</td>
<td>33.19</td>
<td>19.08</td>
</tr>
<tr>
<td>DCSS3</td>
<td></td>
<td>0.875</td>
<td>300</td>
<td>-</td>
<td>44.10</td>
<td>20.61</td>
</tr>
<tr>
<td>DCSS4</td>
<td></td>
<td>0.859</td>
<td>400</td>
<td>-</td>
<td>62.15</td>
<td>22.32</td>
</tr>
</tbody>
</table>
Figure 4-24: Onset of instability presented for CV and DCSS tests at $\sigma'_{vc} = 100, 200$ kPa in a) stress path, b) volumetric strain, c) accumulation of shear strain and d) second-order work variation.

Liquefaction as a form of instability occurs primarily in soils with loose states. The state parameter ($\psi_{cs}$) (Jefferies and Been (1987)), defined as the difference between the consolidation ($e_c$) and critical state ($e_{cs}$) void ratios in a given confinement stress, differentiates between the strain hardening ($\psi_{cs} < 0$), and strain softening ($\psi_{cs} > 0$) behavior of soil. The variations of $\phi'_{yield}$ of CV and DCSS simulations in terms of $e_c$ and $\psi_{cs}$ is plotted in Figure 4-25. As can be seen, $\phi'_{yield}$ decreases as $e_c$ or $\psi_{cs}$ increases.
Similar trends were obtained by Sivathayalan (1994), Riveros and Sadrekarimi (2020b) in an experimental setting on FRS.

![Variations of yield friction angle on void ratio](image1)

![Variations of yield friction angle on state parameter](image2)

**Figure 4-25:** Variations of a) yield friction angle on void ratio, b) yield friction angle on state parameter ($\psi_{cs}$) for CV and DCSS simulations
4.7 Conclusion

In this study, 3D-DEM-based assemblies of DSS stacked-ring device were successfully modeled to study the behavior of sand under monotonic shearing. The microparameters were calibrated to fit the macro response of Fraser river sand. Three types of stress paths including Drained, Constant volume, and Drained constant shear stress were applied to study the instability in drained and undrained conditions. The drained test results illuminated that the frictional angle calculated from beta method ($\beta^\circ$) can predict the mobilized friction angle at the end of simple shearing more accurately. Regarding the constant volume tests, DEM has shown the ability to capture the flow liquefaction behavior after the instability point. Decreasing trends of $\phi'_{yield}$ with $e_c$ and $\psi_{cs}$ were captured for the calibrated material, consistent with the general trends of natural sand deposits.

Drained constant shear tests were performed and compared with constant volume tests in terms of onset of instability. Despite the different stress path applied, various failure criteria such as an abrupt change in accumulation of shear strain, nullification of volumetric strain, second-order work, and $\phi'_{yield}$ showed favorable consensus. It is confirmed that static liquefaction occurs irrespective of the stress path applied.

The evolution of force chains shows the rotation of principal stresses and the generation of large voids at the onset of instability for both drained and undrained stress paths. The variations of coordination number in both cases show a gradual decrease throughout shearing, with an agreement at the onset of instability.
Chapter 5

5 Conclusions

A brief summary of all the concluding remarks obtained from the series of studies is presented in this chapter. Based on the limitations and innovations of this study, ideas for future investigations are proposed.

5.1 Fulfillment of research objectives

In the present study, Discrete Element Method (DEM) was applied as a useful tool to investigate the miscellaneous factors affecting CPT as a penetration problem and to investigate the liquefaction susceptibility and instability analysis of granular materials. This includes in short, simulation of miniature calibration chamber to investigate the effect of various boundaries on CPT measurements in chapter 2, development of a 3D medium under heightened gravitational field to investigate the influence of micro and macro parameters on CPT measurements in chapter 3, and drained and undrained simulation of DSS tests to investigate the instability in granular assemblies in chapter 4. Generally speaking, the following conclusions can be drawn from this study.

Research in chapter 2 sought about the boundary effect observed in calibration chambers from a DEM perspective. Constant stress, constant strain, and constant stiffness boundaries were applied on assemblies with different vertical confinement stress and relative densities. A satisfactory agreement was observed between the results of DEM and experimental miniature calibration chambers. Based on the periodic simulations carried out in DEM, specific correlations were proposed for different boundary conditions to replicate the actual free-field resistances.

Research in chapter 3 focused on the influence of various parameters on CPT measurements. The parameters that were investigated were chosen in terms of micro and macro scale, from inter-particle contact properties to probe geometry. To mimic the conditions observed in the field, a high gravitational field equal to 200g was applied
similar to centrifuge modeling, representing a 40 m soil medium. The results showed that both $q_c$ and $f_s$ are sensitive to relative density, particle shape and particle roughness. Probe wear seems to be an important factor that must be considered in penetration problems. Overall, DEM presented validation as a novel tool to characterize the soil accurately and to investigate the engineering properties in large deformation problems such as CPT in practice.

The objective of chapter 4 is to investigate the instability of granular materials from a micromechanical perspective. This was achieved by simulation of Stacked-ring-Direct Simple Shear test in DEM. A series of drained, constant volume, and drained constant shear stress simulations were carried out on loose assemblies to investigate the behavior of liquefiable material. A unique critical state line was captured based on DEM and previous experimental results. Application of second-order work, accumulation of shear strain, nullification of volumetric strain in defining the onset of instability in drained simulations presented satisfactory agreement with the instability line. It is observed that the liquefaction occurs in a granular assembly irrespective of the stress path applied. Subsequently, using a critical state framework, correlations between yield friction angle ($\phi'_\text{yield}$), void ratio and state parameter were proposed.

### 5.2 Future investigations

The conclusions and limitations drawn from this study triggered the necessity of future investigations in the scope of mesh-free simulations. These possible ideas for the future investigations are listed as below:

I. Within the domains of this study, the effect of particle crushing has been neglected. It is suggested to account for the particle crushing with a failure criterion as it is an important factor in critical state behavior at high confinement stresses or penetration problems.

II. The boundary conditions applied in this series of studies were modeled as rigid. This gives rise to the question whether the application of flexible boundaries
alters the obtained results in miniature chamber tests. For this reason, it is suggested to model flexible boundaries using clusters of particles and compare the results with rigid boundaries.

III. Modeling the actual shape of grains in DEM leads to more accurate stress-strain-volumetric behavior of the material. This can be employed using clump theory coupled with advanced imaging techniques.

IV. All the tests carried out in this study were in a monotonic-quasi-static condition. Cyclic simple shear tests and dynamic cone penetration tests can be employed to investigate the dynamic liquefaction behavior of sand.

V. The effect of boundary conditions on fs measurement has not been investigated in this research due to unreasonable computational efforts. The gap in this scope can be filled with simulation of chambers with significantly high number of spheres.
References


Bolton, M.D., and Gui, M.W. 1993. The study of relative density and boundary effects for cone penetration tests in centrifuge.


Jiang, M., Shen, Z., and Wang, J. 2015b. A novel three-dimensional contact model for


Ng, T.T. 2009. Discrete element method simulations of the critical State of a granular


Rahman, M., Bao, H., and Nguyen, K. 2021. A comparison of critical state behaviour between triaxial and simple shear conditions: A DEM study Une comparaison du comportement à l’état critique entre les conditions de cisaillement triaxiales et simples : une étude DEM.


Robertson, P.K. 2016. Cone penetration test (CPT)-based soil behaviour type (SBT)


Shinohara, K., Oida, M., and Golman, B. 2000. Effect of particle shape on angle of


Appendices

Appendix A-1: Profiles of $q_c$ at $\sigma'^{ve} = 200$ kPa for different $D_{rc}$ and a) BC1, b) BC3, and c) BC5 boundary conditions
Appendix B-2: Profiles of $q_c$ at $\sigma'_{vc} = 100$ kPa for different $D_{rc}$ and a) BC1, b) BC3, and c) BC5 boundary conditions.
Appendix C-3: Profiles of $q_c$ at $\sigma_{ve}^{' \prime} = 50$ kPa for different $D_{rc}$ and a) BC1, b) BC3, and c) BC5 boundary conditions
1 define compute_averagestress
2   global asxx = 0.0
3   global asxy = 0.0
4   global asxz = 0.0
5   global asyx = 0.0
6   global asyy = 0.0
7   global asyz = 0.0
8   global aszx = 0.0
9   global azsy = 0.0
10  global azsz = 0.0
11  loop foreach local contact contact.list("ball-ball")
12   local cforce = contact.force.global(contact)
13   local cl = ball.pos(contact.end2(contact)) - ball.pos(contact.end1(contact))
14   asxx = asxx + comp.x(cforce)*comp.x(cl)
15   asxy = asxy + comp.x(cforce)*comp.y(cl)
16   asxz = asxz + comp.x(cforce)*comp.z(cl)
17   asyx = asyx + comp.y(cforce)*comp.x(cl)
18   asyy = asyy + comp.y(cforce)*comp.y(cl)
19   asyz = asyz + comp.y(cforce)*comp.z(cl)
20   aszx = aszx + comp.z(cforce)*comp.x(cl)
21   aszy = aszy + comp.z(cforce)*comp.y(cl)
22   aszz = aszz + comp.z(cforce)*comp.z(cl)
23  endloop
24  asxx = asxx / (wlz*math.pi*35.e-3*35.0e-3)
25  asxy = asxy / (wlz*math.pi*35.e-3*35.0e-3)
26  asxz = asxz / (wlz*math.pi*35.e-3*35.0e-3)
27  asyx = asyx / (wlz*math.pi*35.e-3*35.0e-3)
28  asyy = asyy / (wlz*math.pi*35.e-3*35.0e-3)
29  asyz = asyz / (wlz*math.pi*35.e-3*35.0e-3)
30  aszx = aszx / (wlz*math.pi*35.e-3*35.0e-3)
31  aszy = aszy / (wlz*math.pi*35.e-3*35.0e-3)
32  aszz = aszz / (wlz*math.pi*35.e-3*35.0e-3)
33 end

Appendix D-3: Computation of the average stresses in the confines of the DSS assembly
Appendix E-3: Radius Expansion Method (REM) used in the generation of some dense assemblies

```plaintext
1 define radius_expansion
2   p_required=10000.0
3   p_limit=0.5*p_required
4   alpha=0.00001
5   co_num=0.0
6   m = measure.find(1)
7   f2=0.0
8   sum=1.0
9   alpha0=0.0
10 loop while math.abs(f2) < p_required
11   command
12       cycle 1
13   endcommand
14   f = measure.stress.xx(m)
15   f0 = measure.stress.yy(m)
16   f1 = measure.stress.zz(m)
17   f2=(f0+f+f1)/3
18   co_num= measure.coordination(m)
19   if math.abs(f2) > p_limit
20       alpha=0.00001
21   else
22       loop while mech.solve("aratio") > 0.01 & math.abs(f2) > p_limit
23         command
24           cycle 1
25         endcommand
26         f = measure.stress.xx(m)
27         f0 = measure.stress.yy(m)
28         f1 = measure.stress.zz(m)
29         f2=(f0+f+f1)/3
30         co_num = measure.coordination(m)
31       end_loop
32   end_if
33   loop foreach b ball.list
34       ball.radius(b)=ball.radius(b)*(1+alpha)
35   end_loop
36   sum=sum*(1+alpha)
37   alpha0=sum
38   poro=measure.porosity(m)
39   end
40 @radius_expansion
41
42
```
Curriculum Vitae

Name: Seyedshayan Hashemi

Post-secondary Education and Degrees:
Amirkabir University of Technology (Tehran Polytechnic)
Tehran, Iran
2011-2015 B.ASc (Civil and Environmental Engineering).

The University of Western Ontario
London, Ontario, Canada
2019-2021 M.ESc.

Honours and Awards:
Western Graduate Research Scholarship
2019-2021

Related Work Experience:
Teaching Assistant
The University of Western Ontario
2019-2021

Research Assistant
Amirkabir University of Technology (Tehran Polytechnic)
Tehran, Iran
2015-2018