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THREE-DIMENSIONAL DEM SIMULATIONS OF MONOTONIC JACKING IN SAND

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Abstract

Understanding the soil responses during monotonic jacking can help improve the estimation of axial capacity in pile foundation design. To examine the soil responses in terms of strain and stress distributions, stress paths, the movement of particles and contact force mobilization during monotonic jacking, a three-dimensional simulation of a centrifuge model pile test was performed using the discrete element method (DEM). The simulation results show great resemblance to the measurements from the centrifuge model pile test. This suggests that our proposed three-dimensional DEM simulation framework is capable of giving accurate estimations of both the shaft and base resistance, especially the latter. The distribution of incremental deviatoric strain $d\varepsilon_q$ indicates the formation of a shear band in the shoulder of the ‘nose cone’ that is beneath the pile base. Based on this, the soil mass can be divided into three zones, i.e., the ‘nose cone’ (zone I), the shear band (zone II) and the surrounding soil beyond the shear band (zone III). The distributions of the radial stress σ_r' , hoop stress σ_θ' , vertical stress σ_v' and shear stress τ_{rv}' are in different modes and high-gradient distributions of mean stress p' and deviatoric stress q are found in zone II. As for the stress path, the surrounding soil experiences four phases in terms of changes in p' and q during monotonic jacking, and the change in the soil stress state decreases with increasing distance from the pile centerline. From a microscopic point of view, the particles in the shear band rotate strongly in a similar direction, fully mobilizing the frictions at the associated contacts. This provides a micromechanical explanation for the soil failure during monotonic jacking.

Keywords DEM • monotonic jacking • deviatoric strain • stress path • friction mobilization

1 Introduction

Monotonic jacking, i.e., penetrating a pile or rod into the subsoil monotonically, is an installation method adopted in the lab and in practice, e.g., in cone penetration tests (CPTs) and model CPT-cone penetration tests in calibration chambers [1]. Even though cyclic jacking or driving rather than monotonic jacking is generally used to install a jacked or driven pile in the field [2], understanding the process of monotonic jacking is relevant to the determination of the axial capacity of jacked or driven piles. Let us consider the process of a static load test, which is widely used to determine the pile capacity. The base resistance of a pile increases with increasing displacement of the pile. Steady state conditions can be reached after large displacement (4 – 10 pile diameters for zero residual stress), with the base resistance approaching the cone resistance obtained from a monotonic jacking process — CPT test, after appropriate averaging of the cone resistance to reflect the larger size of the pile [3]. This suggests monotonic jacking can reproduce the steady state conditions observed in static load tests. The fact that the ultimate pile base resistance can be estimated from the cone resistance based on semi-empirical equations [4-6] also supports this suggestion. Hence, understanding the steady state during monotonic jacking can help improve the estimation of axial capacity.

Several theories have been proposed to characterize monotonic jacking. The two most widely accepted theories are the bearing capacity theory which treats the installation process as the collapsing of the soil mass in the assumed failure zone [7-10], and the cavity expansion theory which describes the process as one of cavity creation and expansion [11-15]. However, due to the simplifications and assumptions involved, the theoretical approaches may give unrealistic soil behavior including

incorrect strain and stress responses, especially if the jacking is performed in sand [16-18].

To gain insights into the soil behavior during monotonic jacking, several experimental investigations have been conducted. Model pile tests have been performed in centrifuge to study monotonic jacking [19-22]. However, due to the restrictions of current techniques for measuring the soil stress in geo-laboratories [18], the soil stress state at a specific penetration depth and the stress path during the whole penetration process have not been examined. In addition, White and Bolton [23] carried out plane-strain calibration chamber tests. They observed that a ‘nose cone’, i.e., a highly compressed region whose core was stationary relative to the pile, formed beneath the pile base. Besides, several slip planes located at the shoulders of the ‘nose cone’ could be identified. But as the plane strain condition adopted in their experiment caused soil movements to extend further from the pile compared with that in field conditions, the experimental observations need to be verified under axisymmetric conditions. In addition, how do the particles at the shoulders of the ‘nose cone’ interact with each other in terms of the relative movement and the contact force mobilization? This question remains to be answered to shed light on the soil failure mechanism from a micromechanical perspective.

Due to the ease of obtaining the values of stress and strain as well as elucidating the micromechanical mechanisms using the discrete element method (DEM), DEM simulations of monotonic jacking have been performed. However, most of the previous studies [24-26] were based on two-dimensional (2D) simulations. Hence, the comparison between the simulation results and experimental results remained qualitative rather than quantitative [27]. As for the contact model used in these studies, no rolling resistance was applied at the particle contacts. This might

lead to large unrealistic particle rotations and an incorrect response of the surrounding soil at both the macroscopic and microscopic scales [28]. In addition to 2D simulations, three-dimensional (3D) simulations of monotonic jacking have also been reported recently [27, 29]. In these simulations, particle rotation was inhibited in an attempt to capture rolling resistance. Even though the macroscale responses, e.g., stress-strain relations in triaxial tests, could be reproduced, the microscale responses, e.g., particle movement, might be questionable. Moreover, in both the previous 2D and 3D simulations, particle scale tests were not taken into consideration when determining the parameters used in the contact models. Therefore, a 3D simulation of monotonic jacking with an appropriate contact model and carefully determined parameters is needed.

The main objective of this paper is thus to construct a 3D DEM framework for simulating monotonic jacking with a particular emphasis on selecting an appropriate contact model and parameter calibration, and then to examine the penetration mechanisms involved from both macromechanical and micromechanical perspectives. A DEM simulation was carried out to simulate the centrifuge model pile test published by Klotz and Coop [22]. The simulation approach was verified by comparing the resistance in the DEM simulation and that in the centrifuge test. Afterwards, the simulation results reveal the macromechanical and micromechanical soil responses, including the strain and stress distributions, stress paths, the movement of particles and contact force mobilization.

2 Details of the DEM Simulations

2.1 Contact model

The contact model defines the contact force-displacement behavior. For simplicity, a 2D assembly of particles is used here to show the contact behavior. The relationships can be easily extended to describe the contact behavior of a 3D assembly.

As shown in Fig. 1a, the relative displacement in the normal direction is given by the overlap U^n of the two entities. Fig. 1b gives the incremental relative displacement in the tangential direction from time t to $t + dt$. The contact point changes from point C to C' , and the material points change from point C to C_1' and C_2' at particles 1 and 2, respectively. The arc lengths $C'C_1'$ and $C'C_2'$, denoted by da and db , are given by

$$da = r_1(d\theta_1 - d\beta_1) \quad (1)$$

$$db = r_2(d\theta_2 - d\beta_2) \quad (2)$$

where r_1 and r_2 are the radii, $d\theta_1$ and $d\theta_2$ are the rotations of the particles, $d\beta_1$ is the rotation from AC to $A'C'$ on particle 1, and $d\beta_2$ is the rotation from BC to $B'C'$ on particle 2. Note that counterclockwise rotation is defined as positive rotation here.

Based on Bardet [30] and Iwashita and Oda [31], the incremental relative frictional displacement dU_s , rolling displacement dU_r and rotation $d\theta_r$ can be described by

$$dU_s = \frac{da + db}{2} \quad (3)$$

$$dU_r = \frac{da - db}{2} \quad (4)$$

$$d\theta_r = \frac{dU_r}{R} \quad (5)$$

where R is the equivalent sphere radius of the two entities. In sum, three force-displacement relationships associated with the relative normal displacement U^n , frictional displacement U_s and rotation θ_r should be included in the contact model.

For the contact laws associated with U^n and U_s , the Hertz-Mindlin model is used as it is capable of capturing the stress-dependent response of soil. As illustrated in Fig. 1c, in the normal direction, no tensile force is allowed, and the contact normal force N is given by

$$N = k^n U^n \quad (6)$$

where k^n is the secant stiffness. The stiffness k^n can be obtained by

$$k^n = \left(\frac{2G\sqrt{R}}{3(1-\nu)} \right) \sqrt{U^n} \quad (7)$$

where G and ν indicate the shear modulus and Poisson's ratio of the entities, respectively. As illustrated in Fig. 1d, in the tangential direction, the incremental friction dT is given by

$$dT = k^s dU_s \quad (8)$$

where k^s is the tangent stiffness. The stiffness k^s can be obtained by

$$k^s = \left(\frac{2\sqrt[3]{3G^2(1-\nu)R}}{2-\nu} \right) \sqrt[3]{|N|} \quad (9)$$

In addition, the magnitude of the shear force T is restricted to a maximum allowable value to characterize the slip behavior between particles, which can be described by

$$|T| \leq \mu |N| \quad (10)$$

where μ is the inter-particle friction coefficient. It is worth noting that the Hertzian response [32] described by equations (6) and (7) is not consistent with the results of particle scale compression tests with real soil particles [33]. As shown in Fig. 2, the initial response is significantly softer and more plastic than previously believed, and a Hertzian response only exists after a threshold load N_{GT} is reached. Based on DEM simulation tests, the threshold load N_{GT} cannot be reached for most engineering applications [34]. Therefore, a smaller shear modulus G instead of the value obtained from pure elastic responses is selected to account for the much softer response.

As for the relative rotation $d\theta_r$, the rolling resistance M_r , i.e., a pair of moment generated at the contact to hinder the relative rotation, can be triggered [35]. Johnson [36] claimed that M_r can be considered as an elastic response arising from the redistribution of the contact normal forces if θ_r is relatively small, and as a plastic response associated with energy dissipation for a relatively large θ_r . The sources of M_r at a relatively large θ_r can be categorized into five types: (a) micro-slip at the contact interface due to dissimilar elastic constants (e.g., shear modulus G , Poisson's ratio ν) or different curvatures of two contacting bodies where energy is dissipated to overcome the frictional force; (b) plastic deformation within the contacting bodies where the energy dissipation is related to the development of a plastic zone; (c) surface roughness effect where energy is dissipated in surmounting the irregularities and development of the local plastic deformation of asperities [36]; (d) surface adhesion where the breaking of adhesive bonds leads to energy dissipation [37, 38];

and (e) interlocking effect where energy is dissipated to overcome the inter-locking among particles [35, 37-41]. The interlocking effect has a much larger influence than the others for most kinds of sand considering the low-sphericity, angularity and non-adhesivity of sand particles [41].

There are three ways to account for the rolling resistance effect (mainly the interlocking effect): non-spherical or ‘clump’ particles without rolling resistance [42-46], spherical particles with rolling resistance [31, 37, 39, 41, 47-50] and a combination of the two methods, i.e., non-spherical or ‘clump’ particles with rolling resistance [51]. Table 1 summarizes the contact models of the rolling resistance, and the associated elements, i.e., different kinds of ‘rolling spring’, ‘rolling dashpot’ and ‘rolling slider’, are given in Table 2.

As Model B3 (see Table 1) is sufficient for quasi-static problems and has a relatively small computational cost, it is used in this study. As shown in Fig. 1e, the elements ‘Spring-A’ and ‘Slider-A’ (see Table 2) are selected owing to their relatively sound theoretical basis. The incremental rolling resistance dM_r is given by

$$dM_r = -k_r d\theta_r \quad (11)$$

where k_r is the tangent rolling stiffness. The stiffness k_r can be obtained by

$$k_r = 2R|N|J_n \quad (12)$$

where J_n is the rolling stiffness constant. Similar to the friction, M_r is restricted to the maximum value M_r^m , which can be described by

$$|M_r| \leq M_r^m = \mu_r b|N|/2 \quad (13)$$

where b is the width of the contacting area (as illustrated in Fig. 1a) and μ_r is the maximum rolling resistance coefficient.

2.2 Calibration of the parameters

Five parameters, i.e., Poisson's ratio ν , shear modulus G , the inter-particle friction coefficient μ , the rolling stiffness constant J_n and the maximum rolling resistance coefficient μ_r are used in the contact model. In the centrifuge test [22], the testing sand was Leighton Buzzard sand. Particle sizes of 0.15–0.212 mm were used. The particles were of solid quartz and were subangular to angular in shape. Hence, the parameters are determined based on the particle-scale tests [33] and triaxial tests [52] on the same sand.

Table 3 presents the detailed procedures of the calibration. Due to the minor influence of Poisson's ratio ν on the macroscopic behavior [49], ν is set to a typical value 0.2, which is the same as that for quartz crystal [53]. Afterwards, the shear modulus G and the inter-particle friction coefficient μ are estimated according to the particle-scale tests conducted by Cavarretta *et al.* [33]. Based on their experimental results, the ranges of G and μ are 0.5~3 GPa (as illustrated in Fig. 2) and 0.27~0.36 (the friction angle = 15°~20°), respectively. Hence, the initial values of G and μ are set to the average values. Afterwards, the parameters associated with the rolling resistance, i.e., J_n and μ_r , are chosen such that the angle ϕ_{cs} from Klotz and Coop [52] can be reproduced in the simulation by trial and error. After that, G and μ are adjusted to make the curves i.e., stress-strain and volumetric response curves, fit the experimental results. The shear modulus G determines the contact normal and tangential stiffness. Hence, it influences the stress-strain and volumetric responses at relatively small strains, and has a minor effect on the soil response at relatively larger

strains (e.g., at the critical state). In addition, based on the simulations of Lau [49], ϕ_{cs} increases with increasing μ and levels off when μ is about 0.27. Hence, if it has been determined that $\mu > 0.27$ from particle-scale tests, adjusting the magnitude of μ will not change ϕ_{cs} . Therefore, G and μ are chosen such that reasonable stress-strain and volumetric responses are achieved in the simulation. This action ensures that ϕ_{cs} is reasonable.

Table 4 presents the parameters determined from the calibration procedure and the sample properties of the DEM simulations of triaxial tests. As illustrated in Figs. 3a and 3b, the DEM simulations (i.e., SIM-1 and SIM-2) reproduce both the stress-strain and volumetric responses of the experimental tests (i.e., LBS-8 and LBS-11) from Klotz and Coop [52]. It is worth noting that the trend of SIM-2 levels off at relatively large strains. Even though the trend is slightly different from that of LBS-8, the simulation result seems more reasonable considering that the critical state can be reached at or before 30% deviatoric strain generally [54]. In addition, the critical state line in the $p'-q$ space is verified in Fig. 3c, indicating that the value of ϕ_{cs} can be reproduced accurately in the simulations regardless of the stress level.

2.3 Simulation setup and procedures

One DEM simulation was conducted to simulate the centrifuge model test denoted by CLBS17 in the paper of Klotz and Coop [22]. As illustrated in Fig. 4, the soil assembly, comprising 608,088 particles, was accommodated in a container composed of one base wall and 25 small cylindrical walls. The particle size and contact model parameters in the simulation of CLBS17 are the same as those listed in Table 4, and a summary of the sample properties of the centrifuge test and the simulation is given in Table 5.

Previous studies have found that the soil-pile interaction is highly influenced by the boundary conditions [19-22]. Based on Salgado *et al.* [1], it is suitable to use constant pressure side boundary and rigid (no displacement) bottom boundary for the penetration problems. Guided by Jiang *et al.* [18], the constant pressure boundary was achieved by adjusting the radii of the side walls (as illustrated in Fig. 4) using a servo-control algorithm in this study. The bottom wall (as illustrated in Fig. 4) was set as a fixed rigid boundary. Both the sample diameter and the minimum clearance from the pile base to the bottom boundary were set as $12D_p$, where D_p was the pile diameter. According to Yang [55], the influence zone of the pile was about $5D_p$ from the pile shaft. Hence, the sample size was large enough to include the influence zone.

Guided by the centrifuge test, soil particles were generated using the radius expansion method, and then the whole system was accelerated to 2000g to consolidate the sample. After that, a cylindrical pile with a diameter of D_p was jacked into the sample at a speed of $\sim 1.5 \times 10^{-4}$ mm/dt until the penetration depth reached $12D_p$. Changes in the soil conditions in terms of stress, strain, particle movements and contact forces were monitored continuously using the measurement spheres distributed in one section (i.e. x - z plane in Fig. 4) of the sample. To capture the high-gradient field in the zone close to the pile toe, smaller measurement spheres with a diameter of $0.2D_p$ were distributed evenly in the near zone close to the pile toe, while larger measurement spheres with a diameter of $0.5D_p$ were used outside the near zone. Meanwhile, changes in radii of the side walls were monitored to rule out any boundary effects.

3 Results and discussions

3.1 Overview

Before pile installation, both the horizontal and vertical stresses, i.e., σ_{h0} and σ_{v0} , increase linearly with depth, and the value K_0 (i.e., σ_{h0}/σ_{v0}) is about 0.5. This is consistent with the condition in the test CLBS17, indicating that the initial stress field of the centrifuge test is reproduced in the simulation. During pile installation, the radius R_b of each side wall changes slightly from the initial value R_{b0} , and the relative change $\Delta R_b/R_{b0}$ is smaller than 1.6%. In addition, the relative change of the pressure on the base wall $\Delta P_b/P_{b0}$ was smaller than 5.85%. The results demonstrate the insignificance of boundary effects in the simulation.

3.2 Base and shaft resistance

Figs. 5a and 5b give the change in unit base resistance q_b and average unit shaft resistance q_s , i.e., the ratio of total friction force on the shaft to the embedded pile length, with the prototype penetration depth. The simulation results show great resemblance to the measurements from the centrifuge model pile test. This suggests the proposed DEM simulation framework, which considers rolling resistance in the contact model and involves a careful calibration based on particle scale and triaxial tests, is capable of giving accurate estimations of both the base and shaft resistance.

3.3 Strain localization

Strain localization, i.e., the localization of deformation into narrow zones of intense shearing, is commonly observed in large strain problems [56]. The phenomenon is believed to be of great importance in understanding the soil failure mechanisms [50]. The field of the incremental deviatoric strain $d\varepsilon_q$ can be used to explain the strain

localization phenomenon [56]. Based on Shrivastava [57], the incremental deviatoric strain $d\varepsilon_q$ is given by

$$d\varepsilon_q = \frac{2}{\sqrt{3}} \sqrt{\frac{1}{6} [(d\varepsilon_{xx} - d\varepsilon_{yy})^2 + (d\varepsilon_{xx} - d\varepsilon_{zz})^2 + (d\varepsilon_{yy} - d\varepsilon_{zz})^2] + (d\varepsilon_{xy}^2 + d\varepsilon_{xz}^2 + d\varepsilon_{yz}^2)} \quad (14)$$

where $d\varepsilon_{ij}$ is the incremental strain tensor. In this study, $d\varepsilon_{ij}$ is the product of the strain rate tensor recorded by the measurement spheres and the time step dt .

Fig. 6a gives the contour images of $d\varepsilon_q$ at different penetration depths. Note that all the values are normalized by the maximum value $(d\varepsilon_q)_{\max}$ in the whole monitoring area at a penetration depth of $12D_p$ to ease comparison. The figure demonstrates a minor change in the distribution mode of $d\varepsilon_q$ with penetration depth. As shown in Fig. 6b, the soil mass can be divided into three zones. Zone I is the ‘nose cone’ beneath the pile toe where $d\varepsilon_q$ remains at a moderate level. Inside the shoulders of zone I, $d\varepsilon_q$ reaches a much higher level, indicating that localizations of deviatoric strain form shear banding in zone II. Beyond zone II, $d\varepsilon_q$ decreases quickly and ultimately reaches a small value in what is referred to as zone III. This is similar to the observations made in the test conducted in a plane strain chamber by White and Bolton [23]. In addition, contours with small $d\varepsilon_q$ (e.g., smaller than 0.01 or 0.001) form spherical surfaces. This suggests that the soil responses in the zone away from the pile toe can be modeled using the spherical cavity expansion method.

3.4 Stress state

At a certain penetration depth, the stress field can be obtained using the distributed measurement spheres. The stress tensor recorded by a measurement sphere is σ_{ij}' , $i = x, y, z$; $j = x, y, z$. Due to the axisymmetric conditions during monotonic jacking, the

stress state of the surrounding soil can be described using the radial stress σ_r' , hoop stress σ_θ' , vertical stress σ_v' and shear stress τ_{rv}' . These stresses can be derived from the stress tensor σ_{ij}' , $i = r, \theta, v$; $j = r, \theta, v$, in a cylindrical coordinate system (see Fig. 4) based on the transformation rules. In addition, the mean effective stress p' and deviatoric stress q are given by

$$p' = \frac{1}{3}(\sigma_{xx}' + \sigma_{yy}' + \sigma_{zz}') \quad (15)$$

$$q = \sqrt{\frac{1}{2}[(\sigma_{xx}' - \sigma_{yy}')^2 + (\sigma_{xx}' - \sigma_{zz}')^2 + (\sigma_{yy}' - \sigma_{zz}')^2] + 3(\sigma_{xy}'^2 + \sigma_{xz}'^2 + \sigma_{yz}'^2)} \quad (16)$$

Fig. 7 presents the associated stress contours at a penetration depth of $12D_p$ and demonstrates the different modes of stress distribution in the surrounding soil. The contour of shear stress τ_{rv}' is presented in Fig. 7a. Considering that there is no shear stress τ_{rv}' in the soil at the initial state (before pile installation), the presence of τ_{rv}' indicates the principal stress rotation during monotonic jacking. As for the distribution of τ_{rv}' , the maximum value is found inside the shoulders of the ‘nose cone’ (i.e., zone II), which is consistent with the formation of a shear band in this zone as illustrated in Fig. 6a. The value decays gradually in a downward diagonal direction (as shown by the dashed arrow in the figure), while the decay along the orthogonal direction is much steeper. Hence, τ_{rv}' is concentrated in a narrow zone in the surrounding soil. As illustrated in Fig. 7b, the maximum radial stress σ_r' is found near the tip of zone I, and σ_r' decays with x and z at a similar rate. The smallest gradient occurs in a downward diagonal direction (as shown by the dashed arrow in the figure). Another horizontal stress, i.e., hoop stress σ_θ' , is presented in Fig. 7c. The value is slightly smaller than σ_r' , and its distribution mode is similar to that of σ_r' . As for the

vertical stress σ_v' (as illustrated in Fig. 7d), the soil in zone I exhibits the maximum value. A very steep decay is shown with x and the rate is larger than that of the horizontal stresses, i.e., σ_r' and σ_θ' . Compared with the decay with x , the decay with z is much gentler and seems to be the gentlest one. In addition, Figs. 7e and 7f show the contours of p' and q , respectively. The value of p' is quite large in zone I, which supports the speculation that zone I is highly compressed given by White and Bolton [23]. Moreover, high-gradient distributions of p' and q are found in zone II. As shown in Fig. 7e, the magnitude of p' reduces from 7000 kPa at point P1 on the boundary between zones I and II to 2000 kPa at point P2 on the boundary between zones II and III. Similarly, the magnitude of q reduces from 10,000 kPa at point Q1 to 2000 kPa at point Q2 in Fig. 7f.

3.5 Stress path

The change in the soil stress state during monotonic jacking has been discussed in several studies [24-26]. Since 2D DEM simulations were used in these studies, the stress state was described using three components — normal stresses in the two directions, i.e., σ_x' and σ_z' , and shear stress τ_{xz}' . This is different from the situation in 3D simulations, where the stress state is more similar to the condition in the field and described using the radial stress σ_r' , hoop stress σ_θ' , vertical stress σ_v' and shear stress τ_{rv}' . Hence, the change in the stress state is discussed again in this study by drawing the stress path using mean effective stress p' and the deviatoric stress q .

Fig. 8a gives the change in the ratio q/p' with the prototype penetration depth observed by the two measurement spheres MS1 ($1.5D_p$, $6D_p$) and MS2 ($2.0D_p$, $6D_p$) with a diameter of $0.5D_p$, the locations of which are also shown in the figure. In parallel, Fig. 8b presents the stress path in p' - q space. Basically, the surrounding soil

experiences a cycle of loading and unloading during monotonic jacking. The whole process can be divided into four phases, and the associated transition points observed by MS1 are also indicated in Figs. 8a and 8b. Initially, in Phase-AB, the values of p' , q and q/p' increase with increasing penetration depth, and the stress path extends toward the critical state line obtained from triaxial tests (see Fig. 3). Then, in Phase-BC, p' and q keep increasing, whereas the ratio q/p' decreases, with increasing penetration depth. Hence, the stress path moves away from the critical state line. In the next phase (i.e., Phase-CD), p' and q start to decrease with increasing penetration depth and the ratio q/p' continues to decrease, implying unloading. An interesting point is that the unloading process starts before the pile base reaches the measurement sphere. This can be explained using Figs. 7e and 7f. As illustrated in the figures, when the soil element flows upward from S1 to S2, p' and q of the soil element reach their maximum values before the pile base reaches the same depth as the soil element. The change in the stress state resembles that during monotonic jacking. Hence, the unloading process starts before the pile base reaches the same depth as the soil element. In the last phase (i.e., Phase-DE), a minor change in the stress state occurs. To summarize the four phases, the typical change in the stress state in a certain soil element with an embedded depth of d is given in Fig. 8c. The soil element experiences four phases in terms of changes in p' , q and q/p' when the pile toe advances from point D_A to D_E . The unloading process starts at point D_C where p' and q begin to decrease with increasing penetration depth. This occurs before the pile toe reaches the same depth as the soil element (as illustrated in Fig. 8c, the distance from D_A to D_C is smaller than d , i.e., $\overline{D_AD_C} < d$). In addition, as illustrated in Figs. 8a and 8b, comparison of the two stress paths observed by MS1 and MS2 demonstrates that the

change in the soil stress state decreases with increasing distance from the pile centerline.

3.6 Micromechanical insights

Fig. 9a gives the micro-structure of the soil near the pile base at a penetration depth of 23.7 m. This provides the micromechanical insights of the distribution modes of the stresses (as illustrated in Fig. 7). The strong force chains basically stretch sideward and downward in the surrounding soil, unlike in the initial state when the strongest force chains stretch downward only. Hence, the principal stresses rotate, which is consistent with the occurrence of τ_{rv}' . In addition, the load on the soil beneath the pile base is transferred along the direction of stretching of the strong force chains. Hence, τ_{rv}' increases in the transfer zone, and decays gently along the stretching direction (as illustrated in Fig. 7a).

To understand details of the particle movements and the contact force mobilization, a force chain FC-23.7 is selected (as shown in Fig. 9a). The coordinates of the particle centers are presented in Fig. 9b using the prototype radial distance from the centerline and the prototype depth (as illustrated with the open squares). To ease the description, the particles are denoted by P-1, P-2, ..., P-12, and the contacts are referred to as C1-2, C2-3, ..., C11-12. For example, C1-2 is the contact between P-1 and P-2. To show the movements of the particle centers, the locations of the same particles at a penetration depth of 23.3 m are also included in the figure (as illustrated with the open circles in Fig. 9b). As shown with the small arrows in Fig. 9b, particles in zone I move almost vertically, while those in zone III move in a downward diagonal direction along the stretching direction of the force chain. A significant

change in the movement direction occurs in zone II. Hence, intense shearing takes place in this area and a shear band forms (as illustrated in Fig. 6a).

Taking the assembly of P-5 and P-6 as an example, Fig. 10a presents a schematic drawing of the relative particle rotation. The angular velocity ω of a particle is described by a vector aligned with the rotation axis. The direction of the vector is taken as the one that ensures the right-hand rule can be applied. The value α_ω is defined as the included angle between the two vectors ω_{P-5} and ω_{P-6} . As shown in Fig. 10b, α_ω is zero if the two particles both rotate along the same axis and the vectors ω_{P-5} and ω_{P-6} point in the same direction, while α_ω is 180° if the two vectors point in opposite directions. For simplicity, the included angle α_ω is treated as a value at the contact. As illustrated in Fig. 11a, the particles in zone II, i.e., P-4, P-5, P-6 and P-7, rotate strongly, while the associated included angles α_ω at the contacts C3-4, C4-5, C5-6 and C6-7 are very small. This implies that the particles in the shear band rotate in a similar direction. This response is similar to that of the shear band in the biaxial tests of Iwashita and Oda [50]. The direct result of the particle rotation mode is that the relative rotational displacement dU_r develops slowly but the relative frictional displacement dU_s develops rapidly. Hence, the friction T and the rolling resistance M_r are mobilized to different degrees. Fig. 11b presents the ratios $|T|/(\mu|N|)$ and $|M_r|/(M_r^m)$ at the contacts in FC-23.7. For the contacts C3-4 ~ C6-7 in zone II, the inter-particle friction is almost completely mobilized while the degree of mobilization of rolling resistance is very low. Therefore, from a microscopic point of view, the soil failure mechanism during monotonic jacking can be attributed to the full mobilization of the friction between the particles in the shear band.

4 Conclusions

In this study, a three-dimensional DEM simulation of a centrifuge model pile test was performed to construct a DEM simulation framework for estimating the resistance during monotonic jacking and to examine the penetration mechanisms involved from both macromechanical and micromechanical perspectives. The salient findings are as follows.

The simulation results show great resemblance to the measurements from the centrifuge test. This suggests that our proposed three-dimensional DEM simulation framework, which considers rolling resistance in the contact model and involves a careful calibration based on particle scale and triaxial tests, is capable of giving accurate estimations of both the base and shaft resistance, especially the latter.

The distribution of incremental deviatoric strain $d\varepsilon_q$ demonstrates localizations of $d\varepsilon_q$ and the formation of a shear band. Based on this, the soil mass can be divided into three zones, i.e., the ‘nose cone’ (zone I), the shear band (zone II) and the surrounding soil beyond the shear band (zone III). In the zone far away from the pile, $d\varepsilon_q$ is very small, and the associated contours form spherical surfaces. This verifies the applicability of the spherical cavity expansion method to problems associated with a small $d\varepsilon_q$ zone.

The distributions of radial stress σ_r' , hoop stress σ_θ' , vertical stress σ_v' and shear stress τ_{rv}' are in different modes. The maximum σ_r' is found near the tip of zone I, and σ_r' decays with x and z at a similar rate. A similar mode is also found in the distribution of σ_θ' . As for σ_v' , the soil in zone I exhibits the maximum value, and the decay of σ_v' with z is much gentler than the decay with x . In addition, the maximum

value of τ_{rv}' is found inside the shoulders of the ‘nose cone’ (i.e., zone II), and high-gradient distributions of p' and q are found in Zone II. This is consistent with the formation of a shear band in this zone.

Three-dimensional DEM simulations make it possible to draw the stress path using mean effective stress p' and the deviatoric stress q . The results reveal four phases in the stress path. Initially, the values of p' , q and q/p' increase with increasing penetration depth in Phase-AB. After that, in Phase-BC, the ratio q/p' starts to decrease, while p' and q keep increasing, with increasing penetration depth. In the next phase (i.e., Phase-CD), p' and q also begin to decrease with increasing penetration depth, and this unloading process starts before the pile base reaches the same depth as the soil element. In the last phase (i.e., Phase-DE), a minor change in the stress state occurs. In addition, the change in the soil stress state decreases with increasing distance from the pile centerline.

From a micromechanical perspective, a significant change in the movement direction occurs at the shoulders of ‘nose cone’. Hence, intense shearing takes place in this area and a shear band forms. The particles in the shear band rotate in a similar direction, leading to the relative rotational displacement dU_r developing slowly but the relative frictional displacement dU_s developing rapidly. Therefore, the inter-particle friction is nearly fully mobilized while the degree of mobilization of rolling resistance is very low. Eventually the fully mobilization of friction at the contacts in the shear band leads to the soil failure during monotonic jacking.

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Table 5 Summary of sample properties of the centrifuge test and DEM simulation

Table 1 Summary of models used in the DEM simulations to account for the rolling resistance effect (mainly the interlocking effect)

Model and schematic drawings	Sub-model	References	Remarks (Ai et al. [37])
<p>Model A: Non-spherical or ‘Clump’ particles without rolling resistance at contacts.</p>	Nil.	<p>Chung and Ooi [42] Salot et al. [43] Ferrellec and McDowell [44] Maeda et al. [45] Kozicki and Tejchman [46]</p>	<ul style="list-style-type: none"> • Sufficient for quasi-static and dynamic problems; • Computational cost is relatively large.
<p>Model B: Spherical particles with rolling resistance at contacts.</p>	Model B1: ‘Slider’	<p>Zhou et al. [47] Estrada et al. [41]</p>	<ul style="list-style-type: none"> • Sufficient for quasi-static problems; • Significant torque oscillation may occur for dynamic problems.
	Model B2: ‘Dashpot’	Kondic et al. [48]	<ul style="list-style-type: none"> • Sufficient for dynamic problems; • Not suitable for a problem in which there is a static phase where rolling resistance still exists if the relative rotational velocity is zero.
Model B3: ‘Spring’+‘Slider’	Lau [49]	<ul style="list-style-type: none"> • Sufficient for quasi-static problems; • Significant torque oscillation may occur for dynamic problems.
Model B4: ‘Spring’+‘Dashpot’+‘Slider’	<p>Iwashita and Oda [31, 50] Ai et al. [37] Mohamed and Gutierrez [39]</p>	<ul style="list-style-type: none"> • Sufficient for most quasi-static and dynamic problems.
<p>Model C: Non-spherical or ‘Clump’ particles with rolling resistance at contacts.</p>	Model A and Model B1/B2/B3/B4	<p>Markauskas and Kačianauskas [51] (‘Model A + Model B1’ is used.)</p>	<ul style="list-style-type: none"> • Efficient for quasi-static and/or dynamic problems; • Superior than Model A and B, especially for highly elongated particles; • Computational cost is much larger.

Note: N , T and M_r are the normal force, friction and rolling resistance at contacts respectively; θ_r is the relative rotation (Fig. 1b); M_r^m is the maximum rolling resistance associated with the ‘slider’ (Table 2); C_r and f are the parameters used in the ‘dashpot’ (Table 2); k_r is the rolling stiffness of the ‘spring’ (Table 2).

Table 2 Summary of elements used in Model B

Element	Equations	Parameters	References	Remarks
Rolling Spring	$dM_r = -k_r d\theta_r$ $M_{r,t+\Delta t}^k = M_r^k + dM_r^k$	Spring-A: $k_r = 2R N J_n$	Bardet and Huang [30] Mohamed and Gutierrez [39] Lau [49]	<ul style="list-style-type: none"> Based on basic equations of 2D elastic contact problems and Hertz's theory.
		Spring-B: $k_r = k_s R^2$	Iwashita and Oda [31, 50] Tordesillas et al. [35] Belheine et al. [38]	<ul style="list-style-type: none"> Based on the assumption that torques associated with rolling and sliding displacements are in the same order.
		Spring-C: $k_r = 3k_n \mu_r^2 R^2$	Normal spring constant k_n ; Maximum rolling resistance coefficient μ_r (Slider-A).	<ul style="list-style-type: none"> Based on that the contact is considered as a continuously distributed system of normal and tangential springs.
Rolling Dashpot	$M_{r,t+\Delta t}^d = \begin{cases} -C_r \dot{\theta}_r & \text{if } M_r < M_r^m \\ -f C_r \dot{\theta}_r & \text{if } M_r = M_r^m \end{cases}$	Rolling damping constants C_r and f .	Iwashita and Oda [31, 50] Ai et al. [37]	<ul style="list-style-type: none"> The function of the equations is to stabilize the particles and prevent rolling oscillation if $f=0$; An additional function, i.e., to simulate any physical viscous dissipative interaction, exists if $f>0$.
Rolling Slider	Slider-A: $M_r^m = \mu_r b N / 2$	The maximum rolling stiffness coefficient μ_r .	Sakaguchi et al. [58] Iwashita and Oda [50]	<ul style="list-style-type: none"> The range of μ_r is from 0 to 1, which is the limit of redistribution of contact normal force; μ_r can be larger than 1 to account for geometry effect of realistic particles.
	Slider-B: $M_r^m = M_{\max}$	Threshold value of rolling resistance $M_{\max}$.	Iwashita and Oda [31]	<ul style="list-style-type: none"> A constant value is selected as no essential changes in the microstructure development are observed compared with Slider-A.
	Slider-C: $M_r^m = \alpha R N $, $\alpha = \tan \beta_{\max}$	Maximum inclination angle $\beta_{\max}$.	Estrada et al. [41] Markauskas and Kačianauskas [51] Lau [49]	<ul style="list-style-type: none"> M_r^m is treated as the maximum static rolling resistance.
	Slider-D: $M_r^m = \alpha R N $, $\alpha = f(\psi)$	Dilatancy angle of the trajectory of particle's center ψ .	Estrada et al. [40]	<ul style="list-style-type: none"> Based on equal energy dissipation for a certain travel angle of particles in reality and in simulations. Only solutions for some polygons are available now.

Note: M_r^k is the elastic rolling resistance; θ_r is the relative rotation; k_r is the rolling stiffness (Rolling Spring); N is the normal force; R is the equivalent radius of two contacting bodies (Spring-A); M_r^d is the viscous rolling resistance (Dashpot); M_r^m is the maximum rolling resistance; b is the width of contact area and shown in Fig. 1a (Slider-A); $M_{\max}$ is the threshold value independent of the normal force (Slider-B).

Table 3 Procedures of the calibration approach

Step	Remarks
1. Determine Poisson's ratio ν	Poisson's ratio ν has minor influence on the macroscopic behavior [49]. The value is selected as 0.2 based on experimental tests on quartz crystal.
2. Estimate the ranges of shear modulus G and the inter-particle friction coefficient μ	This is based on the particle-scale tests conducted by Cavarretta <i>et al.</i> [33].
3. Set the initial value of the parameters G and μ	The initial values can be set as the average values of the results from particle-scale tests.
4. Determine the rolling resistance constant J_n and the maximum rolling resistance coefficient μ_r by trial and error	The values of J_n and μ_r at which a reasonable critical state friction angle ϕ_{cs} is obtained in the simulation are selected.
5. Determine the shear modulus G and the inter-particle friction coefficient μ by trial and error	<p>Shear modulus G determines the contact normal and tangential stiffness, hence, the value influences the stress-strain and volumetric responses at relatively small strains, and has a minor effect on the soil response at relatively larger strains (e.g., at critical state).</p> <p>In addition, based on the simulations of Lau [49], ϕ_{cs} increases with increasing μ and levels off when μ is about 0.27. Hence, if $\mu > 0.27$ from particle-scale tests, adjusting the magnitude of μ will not change ϕ_{cs}.</p> <p>Therefore, G and μ are chosen such that reasonable stress-strain and volumetric responses are achieved in the simulation. This action ensures that ϕ_{cs} is reasonable.</p>

Table 4 Triaxial sample properties and parameters used in the simulations

Sample properties and parameters	Value
<i>Contact model parameters</i>	
Shear modulus G	1.0 GPa
Poisson's ratio ν	0.2
Inter-particle friction coefficient μ	0.32
Rolling stiffness coefficient J_n	2
Maximum rolling resistance coefficient μ_r	12
<i>Sample properties</i>	
Largest particle diameter	0.212 mm
Smallest particle diameter	0.150 mm
Mean particle diameter d_{50}	0.172 mm
Particle density	2650 kg/m ³
Particle number in Sim-1 and Sim-2	11, 529
Sample diameter in Sim-1 and Sim-2	$18d_{50}$
Sample height in Sim-1 and Sim-2	$36d_{50}$

Table 5 Summary of sample properties of the centrifuge test and the DEM simulation

Sample properties	DEM simulation	Centrifuge test: CLBS17
Particle number	608, 088	
Time step dt	$\sim 1.5 \times 10^{-7}$ s	
Pile diameter D_p	1 mm	16 mm
Soil mass diameter	12 D_p (Constant pressure side boundary)	19 D_p (Rigid side boundary)
Minimum clearance between pile base and the base boundary	12 D_p (Rigid base boundary)	4 D_p (Rigid base boundary)
g level	2000g	100g
Prototype maximum penetration depth	24 m	37.5 m
Penetration velocity at the model scale	1.0 m/s ($\sim 1.5 \times 10^{-4}$ mm/ dt)	0.1~0.2 mm/s

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- Fig. 1** Contact model: **a** relative displacement in the normal direction; **b** relative displacement in the tangential direction from time t to $t + dt$; **c** contact model in the normal direction; **d** contact model associated with the relative sliding component; **e** contact model associated with the relative rolling component.
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- Fig. 8** Stress path of the surrounding soil: **a** change in q/p' with the prototype penetration depth; **b** stress path in the $p'-q$ space; **c** schematic drawing of the stress change in different penetration phases.

Fig. 9 Micro-structure of the soil close to the pile base: **a** side view of the micro-structure comprising strong force chains; **b** selected force chain FC-23.7 and change of the force chain from a prototype penetration depth of 23.3 m to 23.7 m.

Fig. 10 Definition of the included angle α_ω and the angular velocity ω : **a** schematic drawing of a general particle rotation form; **b** specific particle rotation forms when $\alpha_\omega = 0$ or 180° .

Fig. 11 Particle rotations and contact force mobilization: **a** normalized angular velocity magnitude $|\omega|/|\omega|_{\max}$ and α_ω of the particles in FC-23.7; **b** degree of mobilization of rolling resistance $|M_r|/M_r^m$ and that of friction at contacts in FC-23.7.

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(a)

(b)

(c)

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(a)

(b)

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Fig. 7 Stress contours at a penetration depth of $12D_p$: **a** shear stress τ_{rv}' ; **b** radial stress σ_r' ; **c** hoop stress σ_θ' ; **d** vertical stress σ_v' ; **e** mean effective stress p' ; **f** the deviatoric stress q .

(a)

(b)

(c)

Fig. 8 Stress path of the surrounding soil: **a** change in q/p' with the prototype penetration depth; **b** stress path in the p' - q space; **c** schematic drawing of the stress change in different penetration phases.

(a)

(b)

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(a)

(b)

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(a)

(b)

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