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Numerical Modelling of Die and Unconfined Compactions of Wet Particles

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Abstract

A numerical method, based on the Discrete Element Method (DEM), is developed to simulate the closed-die compaction and unconfined compaction of wet granular materials. Elastic perfectly plastic are assumed for particles, local contacts are characterized by non-linear elastic and linear plastic deformation. The capillary force is explicitly considered. Solid bonds are introduced between contacting particles to account for the strength gain after closed-die compaction. The numerical model is described in detail. We also illustrate how the compact properties such as compressive strength and failure pattern are influenced by the bond strength and compaction pressure, which determine the mechanical and geometrical integrity of compact. The numerical results demonstrate a qualitative agreement with corresponding results from previous theoretical, experimental studies for the trend of stress-strain response and failure patterns under unconfined compaction. This study proves that solid bond model must be taken into account when modelling granular compaction process using DEM method.

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1. Introduction

Compaction of powders is widely used in many industries to manufacture components with sufficient strength [1, 2]. The mechanical strength is an important criterion to evaluate the quality of a formed compact as it is critical to maintaining geometrical and mechanical integrity of the compact in the downstream operations such as coating, packaging and transport. A number of testing methods thus have been developed to assess this property, such as diametric compression for evaluating the tensile strength and unconfined uniaxial compression to determine the compressive (or crushing) strength of a compact [3, 4]. In general, the compact experiences elastic and plastic deformations under compression with the stress inside the compact gradually building up. When a peak value is reached, fracture of the compact occurs and the stress drops down to a residual stress state [5]. Depending on the powder properties and testing conditions, different failure patterns have been observed, such as crack/breaking line and shear band [6]. Theories based on fracture mechanics and bonding mechanisms have been proposed, but so far the failure mechanisms of the compact are not yet well understood.

Considering the macroscopic response in compaction is the integration of the discrete interactions between particles, better knowledge of these interactions at the particle scale can improve our understanding of the failure mechanisms of the compact. In that regards, numerical modelling based on the discrete element method (DEM) is a cost effective way as it allows the discrete nature of particles to be accounted for. The DEM studies on powder compaction have been carried out to characterize mechanical properties of single particle [7, 8], inhomogeneity induced by particle-wall friction [9], the evolution of internal structure [10], the effects of particle shape and particle size [11, 12]. Recently, DEM has been extended to simulate compaction of powders with relative density higher than 0.85 [13]. However, little work has been carried out to link the mechanical response during compaction and the strength of the compact. Moreover, those observed failure patterns [14-16] and underlying mechanisms have not been thoroughly investigated.

This work is thus to develop a DEM model to simulate the die compaction and unconfined compression of wet granular materials. To mimic the brittle feature of compacts under compaction, a beam bonding force model is included in the model. Similar methods have been used in the previous studies to model sand and cemented materials [17-21]. The evolution of microstructure and forces, the strength of the compacts and failure patterns will be analysed. The effects of consolidation pressure and bonding strength on the compact strength are also investigated.

2. DEM model description

Compaction is a slow process, so a GPU based DEM model has been developed to speed up the simulations. For a particle with radius $R_i$ and $m_i$ mass, its translational and rotational motions can be described by Newton’s second law of motion, given by:

$$m_i \frac{dv_i}{dt} = \sum_j (F_{ij}^n + F_{ij}^{cap} + F_{ij}^{tan} + F_{ij}^{bn} + F_{ij}^{bs}) + m_i g$$

(1)

$$I_i \frac{dw_i}{dt} = \sum_j \left( R_i \times F_{ij}^w - \mu_i R_i \cdot F_{ij}^w \right) v_i + \left( T_{ij}^{bn} + T_{ij}^{bs} \right)$$

(2)

where $v_i$, $w_i$, and $I_i$ are, respectively, the translational and angular velocities, and moment of inertial of particle $i$; $R_i$ is a vector pointing from particle centre to contact point. $\mu_i$ is the coefficient of rolling friction. $F_{ij}^n$ and $F_{ij}^t$ are the normal and tangential contact forces, respectively. $F_{ij}^{cap}$, $F_{ij}^{bn}$ and $F_{ij}^{bs}$ represent, respectively, the capillary force and the solid bonding force in the normal and tangential directions. $T_{ij}^{bn}$ and $T_{ij}^{bs}$ represent the normal and tangential torques on particle $i$ caused by solid bonds, as schematically shown in Fig. 1.
i) Contact model

An elastic-perfectly plastic contact model proposed by Thornton et al. [22] was adopted, given by,

\[
F_y = \begin{cases} 
\frac{4}{3} E R^2 \delta^{3/2} & \left( \delta < \delta_v \right) \\
F_y + \pi p_y R \left( \delta - \delta_v \right) & \left( \delta \geq \delta_v \right)
\end{cases}
\]

(3)

where \(\delta\) is the overlap between particle \(i\) and particle \(j\), \(p_y\) is the yielding pressure beyond which the particles deform plastically, \(\delta_v\) and \(F_y\) are the corresponding overlap and force at the onset of the plastic deformation. \(R^*\) and \(E^*\) are the effective radius and Young’s modulus of the two particles. The unloading and reloading processes are assumed elastic.

The tangential contact force is given by [23]

\[
F_{\tau} = \mu_s F_y \left[ 1 - \left(1 - \frac{\xi_{\tau,max}}{\xi_{\tau,max}}\right)^{1.5} \right]
\]

(4)

where \(\mu_s\) is the sliding friction coefficient, \(\xi_{\tau}\) the total tangential displacement of particles during contact. \(\xi_{\tau,max}\) is the threshold value determining the onset of gross sliding and given by \(\xi_{\tau,max} = 3 \mu_s F_y / (16 G^* a)\), where \(G^*\) is the effective shear modulus defined as \(G^* = E^* (1 - \nu) / (4 - 2\nu)\). \(a\) is the radius of the contact area.

ii) Capillary force

The detailed description of the capillary force can be found in the previous study [24]. The following equations were adopted in our model:

\[
F_{\tau} = \begin{cases} 
\frac{2\pi R \gamma \cos \theta}{1 + \frac{1}{2} \left[1 + 2V_L \left( \frac{\pi RS^2}{1 + 2V_L} \right) - S \right]} & (P - P) \\
\frac{4\pi R \gamma \cos \theta}{1 + S \sqrt{\pi R V_L}} & (P - W)
\end{cases}
\]

(5)
where $\gamma$ is the surface tension of liquid. The solid-liquid contact angle $\theta_c$ and the interparticle separation $S$ are defined as indicated in Fig. 1. A minimum separation $S_{\text{min}}$ is adopted to take into account surface roughness. The rupture distance is given as $S_{\text{rupt}} = (1 + 0.5\theta_c) V_L^{1/3}$.

iii) Bonding force

The BPM model proposed by Potyondy and Cundall [21] was adopted to describe the interparticle bonding forces and torques which are calculated incrementally, given by

$$\Delta F_{ij}^{bn} = -k^* A \Delta \delta^*$$
$$\Delta F_{ij}^{bs} = -k^* A \Delta \delta'$$
$$\Delta T_{ij}^{bn} = -k^* J \Delta \theta^*$$
$$\Delta T_{ij}^{bs} = -k^* J \Delta \theta'$$

(6)

where $k^*$ and $k'$ are the bond normal and tangential stiffness. $\Delta \delta^*$, $\Delta \delta'$, $\Delta \theta^*$ and $\Delta \theta'$ are, respectively, the incremental displacements and rotation in the normal and tangential directions. For a bond with radius $R_b$ and length $L_b$, its bonding area $A = \pi R_b^2$, moment of inertia $I = \pi R_b^4/4$ and polar moment of inertia $J = \pi R_b^4/2$. The bonds can break either by tensile or shear stress and the criteria for bond failure are given by,

$$\min \left( \frac{F_{ij}^{bn}}{A} + \frac{T_{ij}^{bn} R_b}{I}, \frac{F_{ij}^{bs}}{A} + \frac{T_{ij}^{bs} R_b}{I} \right) \geq \sigma_b$$

(7)

where $\sigma_b$ is the strength of the bonds. Once broken, these bonds can no longer be restored. In this work, the bonding area is proportional to the contact area between the particles.

3. Simulation conditions

This work simulated the die compaction of particles followed by unconfined compression. The whole procedure included four stages, particle filling, die compaction, unloading/relaxation and unconfined compaction, as shown in Fig. 2.

![Fig. 2 Schematic representation of the processes for the closed-die compaction and the unconfined compaction: (a) particle filling, (b) loading, (c) unloading and relaxation, and (d) unconfined compression](image)

At the filling stage (Fig. 2a), particles were generated randomly by batch inside a cylindrical container and fell down under gravity to form a packed bed. Once the packing was stabled, the upper punch moved downward at a
small, constant velocity to compress the particles (Fig. 2b). After the compact reached a prescribed packing density, the unloading process stared with the punch moving upward until the punch was detached from the compact (Fig. 2c). After a short period of relaxation, the bonding forces were introduced between contacting particles with bonding area the same as contact area. The cylindrical wall was then removed and the punch moved downward for the unconfined compaction.

4. Results and discussion

4.1 Die compaction

Fig. 3a shows a typical die compaction curve in which the pressure acting on the upper punch is plotted against the compact density. At the initial stage of the compaction, the density of the compact increases quickly with little pressure applied from the punch. The increase in density at this stage is mainly due to the rearrangement of the particles with little deformation of the particles [10]. At the end of the stage, all the particles have been locked into their stable positions and cannot move further. So with further increase in pressure, the particles start to deform, resulting in quick increase in pressure. The unloading curve indicates that the unloading process is governed by the elastic recovery. Coordination number (CN) has long been considered as a measurement of local structure. Fig. 3b shows the variation of the mean coordination number during the compaction process. At the initial stage of loading process where the particle rearrangement is dominant, the particles simply change their positions, resulting in a small increase in the mean CN. At the loading stage where the particle deformation is dominant, the mean CN shows a linear increase with packing density.

Fig. 3 (a) A typical pressure-density compaction curve; and (b) the variation of mean coordination number with density.

Compaction not only increases compact density but also causes inhomogeneous density and stress distributions inside the compact. Fig. 4a shows the spatial distribution of density at different stages as marked in Fig. 3a. At stage A with a low density $D = 0.53$, the density distribution is largely homogenous. In the middle of the loading process, the density distribution becomes increasingly inhomogeneous with higher density at the top and lower density at the bottom. This variation of the density along the compaction direction is attributed to the effect of friction between the particles and the die wall. A similar trend of density distribution was also observed for ceramics [2] and pharmaceutical powders [25]. Comparing stages C and D, the density distribution is almost unchanged at the unloading stage.

Fig. 4b shows the structure of normalised force chains at the corresponding stages. At state A, only a small portion of contacts near the punch carries larger forces. At state B, the forces are transmitted from the top to the bottom with vertically aligned pathway and clearly showing force gradients along the axial direction with larger force at the punch propagating downward to transmit the applied pressure. This is different from the force distribution in the particle packing as the applied pressure takes over from gravity as the dominant force. At the final stage of the loading process, the force network reveals a strong force-chain pattern with smaller force clusters.
embedded among them. It is clear that a network of stress path is developed and the applied load is largely transmitted by heavily stressed chains of particles forming a relatively sparse network. After the unloading process, the force distribution decreases significantly as the top punch moving upward. Hence it can be concluded that the force is more sensible to process transition than structure as shown in the density distribution.

Fig. 4 The spatial distributions of (a) density, and (b) normalised contact forces at different stages.

4.2 Unconfined compression

Unconfined compression test is a simple and practical approach to measure the compressive strength of a compact. Fig. 5a shows the typical stress response during the unconfined compaction which leads to relatively stable residual stress state. It is observed that the trend of axial stress is approximately linear up to the peak value of 20 KPa beyond which the failure of the compact occurs. The peak stress is known as the compressive strength of compact. Three main characteristics of the stress-strain response, namely the linear increasing part, peak value and residual stress state, are captured in the simulations. Similar trend are also observed in experimental works, such as pharmaceutical powders [25] and detergent powders [26]. The Young’s modulus of the compact can also be derived from the slope of linear increasing part of the plot, which gives a value of $7 \times 10^5$ Pa.

The failure patterns at different stages as marked in Fig. 5a are shown in Fig. 5b. The broken mechanisms are represented by different colours: red points are the tension-induced breakage for which the bond tensile strength has been exceeded, and yellow points represent shear-induced bond breakage for which the bond shear strength has been exceeded. Before the compact reach its failure point, very few bonds are broken which are distributed uniformly throughout the compact, indicating a relatively intact internal structure. Breakage pattern starts to shown at the peak stress point ($\varepsilon = 3.17\%$) in which the fracture propagates through the compact. With increasing axial strain ($\varepsilon = 3.96\%$), the principal shear band becomes more prominent, indicating an increased bond breakage in the shear band. The principal shear band that cuts across the compact forms over a relatively small strain interval during decreasing macroscopic stress. A secondary shear band located under the principal shear band occurs as the process continues, which is characterized by the decreasing rate of stress drop and bond breakage.
4.3 Effects of compaction pressure and bond strength

Compaction pressure and bonding force are two critical parameters affecting the mechanical strength of compacts. Fig. 6a show the axial stress-strain responses for the compacts formed under different pressures. As expected, increasing compaction pressure increases the compressive strength of the compacts with the peak value increasing from 13KPa to 22KPa. It is also observed that with increasing compaction pressure, the axial strain at the failure point and Young’s modulus of the compact also increase, indicating increasing brittleness of the compact. These trends are in good agreement with the experimental observations obtained by other researchers [27].

Fig. 6b shows the failure patterns of the compact formed with different compaction pressures. The same representation method used in Fig. 5b is adopted here plus the green points represent the intact bonds and blue ones mean that no bond exists. It is noted that as the compaction pressure increases, the distribution of bond breakage varies from throughout the bottom region with small bulging to localized shear bands.
Fig. 7 shows the effect of bond strength on the strength of the compact and failure patterns. Fig. 7a shows the axial stress-strain responses with different bond strengths. Before the failure point, no noticeable difference is observed except for increased peak value with larger bond strength, indicating insensitive pre-peak behaviour with changing bond strength. The difference in the response after the peak values is more significant with sharper drop of stress with increased bond strength, suggesting the compact is more brittle with stronger bonds.

This is also observed from the failure patterns as shown in Fig. 7b. While strain localization occurs for all the cases, the fracture patterns are more clear and localised with larger bond strength. For the small bond strength $\delta_b = 20$KPa, the bond failure occurs throughout the bottom region with no clear shear banding phenomenon. With $\delta_b = 40$KPa, the broken bonds are more localized and mainly occurs near the marked principal shear band. Further increase in bond strength leads to a reduced width of shear bands and an increasing possibility of occurrence for two complementary shear bands. The results therefore indicate that bond strength is important for forming clear and narrowed shear bands.

5. Conclusion

The potential of DEM for studying the compaction behaviour during the die compaction and unconfined compaction has been presented in this work. We have shown the capability to carry out 3-D DEM simulations to obtain the macroscopic and microscopic information. Both the structure and force information during the compaction process has been gathered and analysed for better understanding of compaction process. Coupled with modified bonded-particle model, the physical characteristic of solid bond was taken into account in the measurement of compressive strength during unconfined compaction. The main advantage of proposed DEM model is that it allows the particle properties, moisture content and the effect of plastic deformation on solid bonding being considered. The linear relationship between compaction pressure and compressive strength was observed. The development of strain localization was presented and the factors that affect the appearance of shear banding were identified.

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