

# Modelling the breakage of a spherical agglomerate in a vertically vibrated granular bed

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**Abstract.** The objective of this work is to investigate the deagglomeration of a cohesive cluster in a bed of granular particles subject to vertical vibration using Discrete Element Method-based numerical simulations. The simulation domain is periodic in the gravity normal direction. The bottom wall oscillates with a fixed frequency of 100 Hz. The amplitude is varied over a large range to simulate the bed at different regimes. The top wall is placed at a height ( $2000d$ ) to prevent particle interactions and thereby mimic a semi-infinite domain. Non-cohesive particle interactions are modelled using a linear spring-dashpot approach, while cohesive interactions are described by the Hertz-JKR model. All particles are assumed to be perfectly smooth. The ratio of the maximum base energy to the cohesive energy ( $\phi$ ) is used for classifying the results obtained from DEM simulations. The data from the simulations is analysed to determine the deagglomeration rate. It is found that deagglomeration is a first-order process, with the deagglomeration rate constant exhibiting a log-linear relationship with  $\phi$ .

## 1 Introduction

Granular particles smaller than  $100\mu\text{m}$  tend to agglomerate due to the dominance of cohesive forces over other body forces [1]. Clustering of particles adversely influences flowability of material [2], coating [3], and food processing [4]. Vibro-fluidization is often used for coating of cohesive particles in order to reduce agglomerate formation [5].

The deagglomeration of clusters within a granular bed is particularly relevant for fluidization of cohesive particles [6, 7]. In large systems, particles often form localized agglomerates, surrounded by non-cohesive particles. Vibration, as an external source of energy, is often used to break large agglomerates within the granular bed in order to achieve uniform fluidization. It is also reported in the literature that the breakage of agglomerates depends greatly on the vibrational parameters [8]. Despite this, there is limited investigation into the effect of vibrational energy on the breakage of agglomerates within the bed. While the impact-induced breakage of agglomerates of various shapes and sizes has been extensively reported in the literature [9]. In the present work, we aim to understand the effect of vibrational energy on the de-agglomeration of a cohesive agglomerate within a vibrated bed.

The specific objectives of the current work are :

1. To investigate the effect of the ratio of maximum energy of the vibrating base to the interparticle cohesive energy ( $\phi$ ) on the deagglomeration of a spherical agglomerate within a granular bed.

2. To model the breakage of a spherical agglomerate as a rate process and determine the dependence of the rate constant on  $\phi$ .

To achieve these objectives, discrete element method (DEM) simulations of dry cohesive granular systems are performed using the open-source software LAMMPS.

## 2 Methodology

### 2.1 Simulation domain

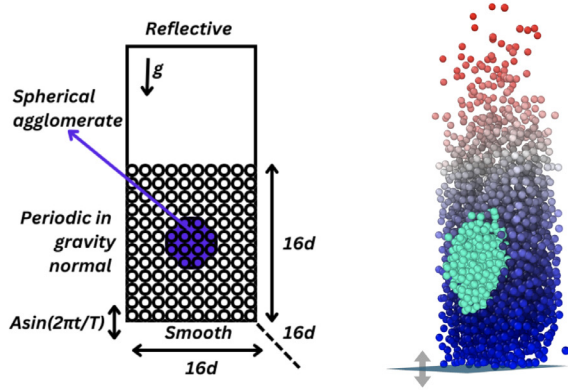
Figure 1 shows the schematic of the simulation domain used for this study. The simulation domain is periodic in the gravity normal direction. The top wall is reflective and placed at a height of  $2000d$ . The bottom wall vibrates sinusoidally with amplitude ( $A$ ) and frequency ( $f$ ) such that the wall position varies as  $y_w = A \sin(2\pi ft)$ . The maximum velocity and energy of the base are  $U_o = 2\pi Af$  and  $4\pi^2 A^2 f^2$ , respectively. The bottom wall is assumed to be smooth and perfectly elastic.

Initially, the system consists of 16 layers of particles arranged within a three-dimensional periodic domain. Each layer contains a  $16 \times 16$  array of particles along the direction normal to gravity, with  $s = d$  where,  $s$  is the interparticle distance and  $d$  is the particle diameter. Particles within a radius of  $2d$  from the particle placed at the center of the bed are considered cohesive, while the remaining particles are non-cohesive.

First, the cohesive particles at the centre of the bed are allowed to interact under the action of cohesive force to form a spherical agglomerate of diameter  $4d$ . In the

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**Figure 1.** (a) Schematic of the simulation domain used in this study. (b) A simulation screenshot showing cohesive agglomerates at the center, with non-cohesive particles color-coded based on kinetic energy, where red indicates the maximum and blue represents the minimum.

agglomerate, each particle is in contact with at least one other particle within the agglomerate. These particles are marked in blue in Fig. 1a. This particle configuration is used as the initial condition for further simulations.

$\phi$  defined as the ratio of maximum energy of the vibrating wall per unit mass ( $4\pi^2 A^2 f^2$ ) to the interparticle cohesive energy per unit mass ( $m$ ) ( $\frac{\pi d^2 \gamma}{m}$ ) is varied between 0.01 and 50. The frequency of vibration and interparticle surface energy is kept fixed at 100 Hz and  $0.25 \text{ mJ m}^{-2}$ . Vibration amplitude is varied between  $0.15d$  to  $11d$  to vary  $\phi$ . The corresponding dimensionless acceleration of the granular bed ( $\Gamma = \frac{4\pi^2 A f^2}{g}$ ) ranges from 0.6 to 60.

The number density of bed particles is maintained constant at  $1.6 \times 10^9 \text{ m}^{-2}$ . Figure 1b shows a typical snapshot of the simulated bed with a cohesive agglomerate.

## 2.2 Discrete Element Method

The interaction between the non-cohesive particles is modelled using the linear spring and dashpot method, such that the contact force in the direction normal to the unit vector joining the centre of particles is given as follows.

$$\vec{F}_{nij} = -k_n \xi_{nij} \hat{r}_{ij} - \gamma_n \vec{V}_{nij} \quad (1)$$

where  $k_n$  and  $\gamma_n$  are the stiffness and viscous dashpot coefficients in the normal direction.

The interaction between cohesive particles is modelled using the Hertz-JKR model, where the contact force in the direction normal to the unit vector joining the centre of particles is

$$\vec{F}_{n,JKR} = \left( \frac{4E_{eff} a^3}{3R_{eff}} - 2\pi a^2 \sqrt{\frac{4\gamma E_{eff}}{\pi a}} \right) \hat{r}_{ij} \quad (2)$$

where  $E_{eff}$  is the effective Young's modulus, and for two spheres of the same material, it is defined as

$E_{eff} = E/(1 - \nu^2)$  with  $\nu$  as the Poisson ratio of the particle. The effective radius is defined as  $R_{eff} = d/4$  and the contact zone radius, denoted as  $a$ , is related to the overlap  $\xi_n$ , such that:

$$\xi_n = a^2/R - 2\sqrt{\pi\gamma a/E_{eff}}. \quad (3)$$

Here,  $\gamma$  represents the surface energy, which quantifies the strength of interparticle cohesion. The interaction between cohesive and non-cohesive particles is modeled using the linear spring-dashpot method. The material properties and DEM input parameters, adopted from [10], are summarized in Table 1.

**Table 1.** Material properties of the particles used in the DEM simulation.

Particle Property	Value
Diameter, m	$10^{-4}$
Linear Spring Constant, ( $mg/d$ )	$2 \times 10^7$
Coefficient of Restitution	0.9
Young's Modulus, Pa	$10^8$
Poisson Ratio	0.3
Density, $\text{kg/m}^3$	1500
Surface Energy, $\text{mJ/m}^2$	0.25

## 2.3 Analysis of DEM data

Position and linear velocities of non-cohesive and cohesive particles from the DEM simulation are further analysed to determine the evolution of cluster size and the centre of mass of the granular bed.

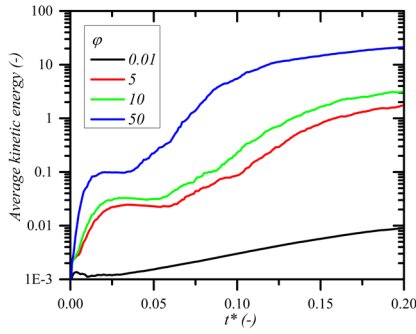
A pair of particles ( $i, j$ ) are considered to be in contact if  $\vec{r}_{ij} \leq d$ , where  $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$  and  $\vec{r}_{i,j}$  are the position vectors of particles  $i, j$  respectively. A particle is considered part of an existing cluster if it is in contact with any other particle in the cluster. The cluster size is determined and plotted as a function of time. The centre of mass (COM) of the granular bed is plotted against time. For each timestep, centre of mass is determined by taking the average of the vertical component  $z$  of all particles. Simulation time is normalized with the time period ( $T$ ) of the vibration (or  $1/f$ ) such that  $t^* = t/T$ .  $\phi$  is used as the main parameter for analysing the simulation results.

## 3 Results

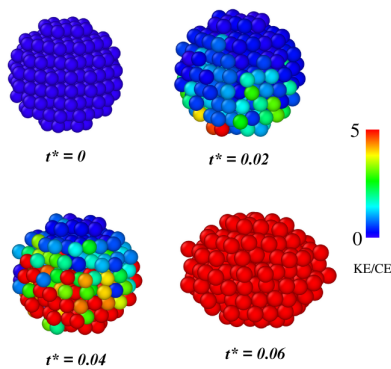
### 3.1 Kinetic energy of particles

The average kinetic energy of all particles within the agglomerates, normalized by the surface energy of the particles ( $4\pi d^2 \gamma$ ), is plotted in Fig. 2 for different values of  $\phi$ . It is observed that the kinetic energy of the particles within the agglomerates gradually increases, resulting in deagglomeration. For  $\phi \geq 5$ , the kinetic energy of the particles within the agglomerates exceeds the interparticle surface energy.

Snapshots of spherical agglomerate (within the granular bed) from the simulation are shown at four different



**Figure 2.** Average kinetic energy of particles normalised with the surface energy within the agglomerate as a function of time for different values of  $\phi$ .



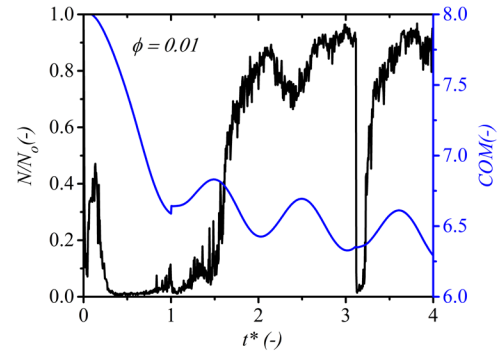
**Figure 3.** Screenshots of particles on the agglomerate surface within the vibrated bed are shown at various time instances ( $t^* = t/T$ ) for  $\phi = 10$ . The color indicates the ratio of each particle's kinetic energy to its cohesive energy.

timesteps in Figure 3 for  $\phi = 10$ . Particles are coloured as per the magnitude of the ratio of kinetic energy ( $1/2mv^2$ ) to the cohesive energy ( $\pi d^2\gamma$ ). At  $t^* = 0$ , particles are observed to be stuck together with negligibly small kinetic energy. As time progresses, particles at the bottom of the agglomerates begin to gain energy due to energy transfer from the non-cohesive bed particles. By  $t^* = 0.06$ , the particles within the spherical agglomerate have gained energy up to five times their cohesive energy, leading to complete deagglomeration.

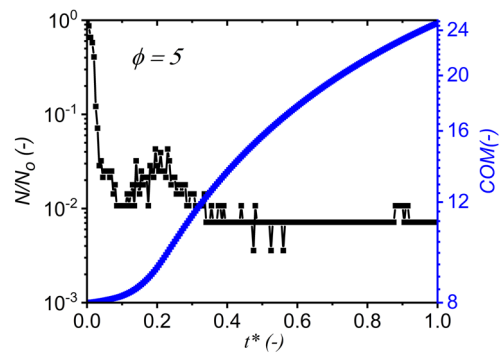
### 3.2 Effect of vibration

The effect of the ratio of maximum energy of the vibrating wall to the interparticle cohesive energy ( $\phi$ ) on the cluster size and the expansion of the granular bed is investigated.

Figure 4 shows the evolution of the centre of mass (normalized by the particle diameter) of the granular bed and the cluster size for  $\Gamma = 0.6$  and  $\phi = 0.01$ . The scaled Centre of Mass of the bed shows an initial drop followed by a periodic motion. The initial reduction in the bed COM is due to the collapse of the bed under its own weight. The subsequent oscillation of the centre of mass indicates a periodic *en-block* motion of the bed. Figure 4 also plots  $\frac{N}{N_0}$  vs time, where  $N_0$  is the initial number of



**Figure 4.** Cluster size of the spherical agglomerate and the centre of mass of the granular bed for  $\phi = 0.01$

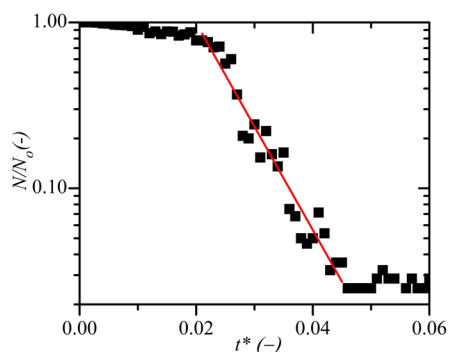


**Figure 5.** Cluster size of the spherical agglomerate and the centre of mass of the granular bed for  $\phi = 5$ .

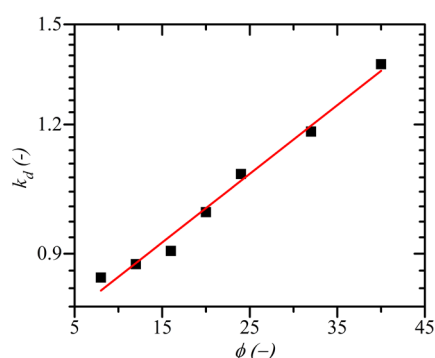
particles and  $N$  is the current number of particles in the agglomerate. The initial deagglomeration results from the collapse of the bed under its own weight. Subsequently, re-agglomeration occurs as the bed exhibits block-like motion. In this phase, particles within the agglomerate remain held together by the forces exerted by neighbouring bed particles. However, it is observed that the particles re-agglomerate, eventually reaching their original size. The sudden decrease in cluster size at the beginning of the third vibration cycle is likely caused by the collision between the bed and the vibrating wall at the bottom. Here, the energy of the vibrating wall is insufficient to deagglomerate the particles completely. Since we are mainly interested in the deagglomeration kinetics, where the phenomenon is breakage-dominant, we studied the behaviour for high values of  $\phi$ .

remains unexplained for now, and further analysis may be required to determine whether this behaviour is periodic.

Figure 5 shows the evolution of the cluster size and the centre of mass of the granular bed for  $\phi = 5$ . Here, the centre of mass of the bed increases monotonically from 8 to 24, indicating the expansion of the bed. This expansion leads to the deagglomeration of the spherical agglomerate, evidenced by the sudden drop in cluster size over time. This observation remains consistent even after a larger number of vibrational cycles.



**Figure 6.** Linear fit of the  $N/N_0$  with the simulation time (normalized with the time-period) in log-linear scale for  $\phi = 17$



**Figure 7.** Linear fit of the deagglomeration rate constant  $k_d$  with  $\phi$  in log-linear scale.

### 3.3 Modelling breakage as the rate process

In this section, the evolution of the cluster size normalised with the initial size is plotted with time for  $\phi = 17$  in the log-linear scale (Figure 6). It is observed that a straight line fits well with the breakage phenomenon from  $t^* = 0.02$  until a complete deagglomeration is achieved. This signifies the first-order breakage of the spherical agglomerate inside the granular bed such that  $N/N_0 = -k_d t/T$ , where the slope of the line is deagglomeration rate constant ( $k_d$ ). The same exercise is repeated for other values of  $\phi$  to determine the rate constant  $k_d$  as the function of  $\phi$ . It is determined that  $k_d$  scales exponentially as  $\phi$ , ( $k_d \propto \exp(\phi)$ ), as shown in Figure 7. This indicates that as the maximum energy of the vibrating base increases, the deagglomeration of the spherical agglomerate takes place more quickly. This is anticipated because, at higher values of  $\phi$ , the average kinetic energy of the bed particles increases, leading to a greater transfer of energy from the non-cohesive particles to the cohesive bed. This is consistent with the plot of average kinetic energy of particles within the agglomerate as shown in Fig. 2.

## 4 Conclusion

This study investigates the deagglomeration of a cohesive spherical agglomerate within a vibrated granular bed.

The interaction between cohesive particles is modelled using the Hertz-JKR method, while the contact between non-cohesive particles is modelled using the linear-spring dashpot. The following are the key conclusions of this work:

- For  $\phi = 0.01$ , the energy of the bed particles is insufficient to break the spherical agglomerate present at the centre of the bed. At this energy ratio, the granular bed moves as a single block.
- At a sufficiently high value of  $\phi$  ( $\geq 5$ ), the granular bed behaves similarly to the granular gas. The spherical agglomerate completely disintegrates.
- It is shown that the breakage of a spherical agglomerate within a granular bed follows a first-order kinetics.
- The breakage rate constant scales exponentially with the ratio of the maximum energy of the vibrating base to the interparticle cohesive energy.

This study provides valuable insights into the role of vibrational energy in the breakage of localized agglomerates, demonstrating that the process follows first-order kinetics. The findings can improve our understanding of how vibration influences mixing, segregation, and fluidization in cohesive powders, with potential applications ranging from the dairy industry to battery manufacturing. Additionally, this work can be extended to examine the effects of individual vibrational parameters on the breakage kinetics.

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