EPJ Web of Conferences **140**, 06024 (2017) DOI: 10.1051/epjconf/201714006024
Powders & Grains 2017

Numerical analysis of the effect of particle shape and adhesion on the segregation of powder mixtures

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Abstract. Segregation of granules is an undesired phenomenon in which particles in a mixture separate from each other based on the differences in their physical and chemical properties. It is, therefore, crucial to control the homogeneity of the system by applying appropriate techniques. This requires a fundamental understanding of the underlying mechanisms. In this study, the effect of particle shape and cohesion has been analysed. As a model system prone to segregation, a ternary mixture of particles representing the common ingredients of home washing powders, namely, spray dried detergent powders, tetraacetylethylenediamine, and enzyme placebo (as the minor ingredient) during heap formation is modelled numerically by the Discrete Element Method (DEM) with an aim to investigate the effect of cohesion/adhesion of the minor components on segregation quality. Non-spherical particle shapes are created in DEM using the clumped-sphere method based on their X-ray tomograms. Experimentally, inter particle adhesion is generated by coating the minor ingredient (enzyme placebo) with Polyethylene Glycol 400 (PEG 400). The JKR theory is used to model the cohesion/adhesion of coated enzyme placebo particles in the simulation. Tests are carried out experimentally and simulated numerically by mixing the placebo particles (uncoated and coated) with the other ingredients and pouring them in a test box. The simulation and experimental results are compared qualitatively and quantitatively. It is found that coating the minor ingredient in the mixture reduces segregation significantly while the change in flowability of the system is negligible.

1 Introduction

Segregation of particulate solids is a phenomenon through which the homogeneity of a mixture is deteriorated by the separation of components due to different properties of the particles within the mixture. For instance, particles size, density, shape, and surface condition influence the segregation; therefore, controlling these factors can reduce the segregation effectively [1, 2]. To do so requires a good understanding of their role. In this study we address the effect of interparticle adhesion on the segregation tendency by coating a selected component with a thin layer of liquid to make it sticky
Particles surface condition can have a significant impact on inducing or reducing segregation mainly by influencing the flowability of the particles. Particles flowability is directly linked with the particles surface condition and surface texture [3-6]. The effects of surface condition is manifested in surface properties namely the coefficients of sliding friction and rolling friction and adhesion/cohesion of the particles.

Increasing the cohesivity of the particles by coating with a thin liquid layer is a typical method to reduce the segregation; as cohesive materials have a2 lower flowability [7, 8]. Particles adhesive tendency is expressed by the ratio of surface forces to gravitational force, known as Bond number [9]. Due to their lower momentum and higher Bond number, finer particles are more affected by coating compared to the coarse ones which may lead to their poor flowability or even caking and agglomeration. Nevertheless, making the minor component sticky in a mixture could be a remedy for reducing their segregation; while the flowability of the whole mixture is not significantly affected [10].

In the present study the segregation of a minor component in a ternary mixture of particles during heap formation is simulated using DEM. The particles properties including size, density, shape, and surface properties are measured experimentally and calibrated to be used in DEM. The minor component ingredient is a round enzyme placebo particle which is coated by PEG 400 to manipulate its stickiness. Segregation of the minor ingredients as affected by the coating in the mixture is simulated and analysed.

2 Methodology

DEM simulation of segregation of particles during the heap formation is carried out and compared with the experiment. Fig. 1 depicts the geometry of the test box in

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DOI: 10.1051/epjconf/201714006024

experiment in which the heap formation is simulated. It is highly important in DEM modelling to set appropriate physical and mechanical properties in the model. While this part has been normally simplified or ignored in many previous studies, in this study the real physical parameters are measured and used where possible.

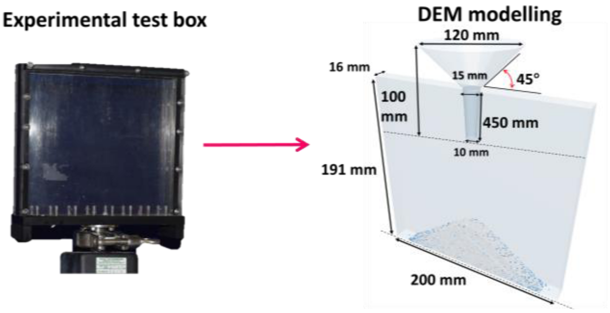

Fig. 1 : Image of the geometry of the test box used in experiment and modelling.

2.1 Particles physical and mechanical properties

Three different particles representing the common ingredients of home washing powders, namely, spray dried detergent powders (commonly referred to as Blown Powder or BP), tetraacetylethylenediamine (TAED), and enzyme granules (placebo used here) are utilized to form a ternary mixture. Particles are in different sieve-cut size ranges based on the mode of their size distribution. Table 1 shows the particles properties such as size, density, shear modulus, coefficients of restitution (COR) and sliding friction (COF) measured experimentally as described in [11, 12].

Table 1. Specifications of the modelling and the materials properties.

Material type	BP	TAED	Enzyme placebo	Perspex
Size (µm)	500-450	850-1000	600-700	----
Particles number	633597	4667	1401	-----
Total mass (g)	28.53	1.71	0.61	-----
Weight Percentage	92	6	2	-----
Particle shape	5-sphere	5-sphere	spherical	Wall
Repose angle	40	36	31	-----
Shear modulus (MPa)	100	100	100	1000
Density (kg/m^3)	780	850	2320	1180
Coefficient of rolling friction	0.10	0.01	0.05	0.01
Poisson's ratio	0.25	0.25	0.25	0.25
COF (BP)	0.62	0.69	0.70	0.42
COF (TAED)	0.69	0.75	0.75	0.36
COF (Placebo)	0.70	0.75	0.75	0.75
COR (BP)	0.20	0.30	0.20	0.28
COR (TAED)	0.30	0.32	0.20	0.32
COR (Placebo)	0.20	0.20	0.10	0.20

2.2 Particles shape

Particles shapes are generated using the clumped-sphere technique and based on the geometries obtained by X-ray tomograms (XRT). ASG software [13] is utilized to generate particle shape by clumping an optimum number of spheres of different sizes [11] as shown in Fig. 2. Generated particles shapes are then used in DEM accompanied with the physical properties of the particles given in section 2.1.

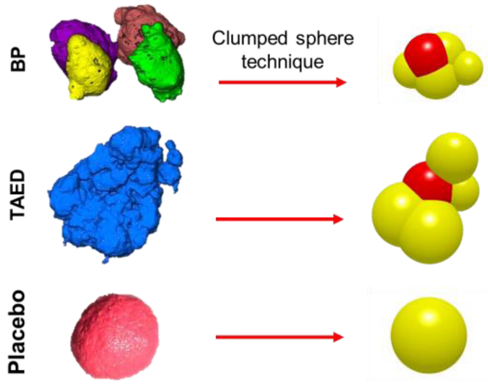

Fig. 2: The clumped spheres representing the real shapes of TAED and placebo particles.

2.3 Numerical modelling and contact models

EDEM 2.7.1 software, provided by DEM Solutions, Edinburgh, UK, is used to model the segregation process. The models used for particles contacts are Hertz-Mindlin [14-16] and JKR [14] by which the effects of collisions and cohesion/adhesion are taken into consideration. Hertz-Mindlin theory is used for calculating the normal and tangential forces during the collision between two particles; where Hertz model [15] calculates the normal impact and Mindlin theory [16] accounts for the tangential force. The details of these models are available elsewhere [17, 18].

Bonding forces in coated materials roots in both surface tension and viscous damping forces. By using the particles surface energy in the JKR model [14] the surface tension forces are taken into consideration and to account for viscous dissipation, low restitution coefficients are selected. To predict a valid surface energy for the particles in JKR model, a dimensionless number, i.e. Cohesion number [19], is used by which the surface energy is predicted for the current system.

$$Coh = \frac{1}{\rho g}\left(\frac{\Gamma^5}{E^{*2}\,R^{*8}}\right)^{1/3} \qquad (1)$$

Lower modulus of elasticity is selected in DEM modelling with the aim of having less computational effort but the cohesion number is kept constant by changing the surface energy. The rest of the parameters in the cohesion number are the same as those of the experiment. Enzyme placebo particles are coated by different mass ratios of PEG 400 and then the repose angle for each coating level is measured experimentally. The equivalent surface energy to obtain the same angle of repose in the modelling is then found by back-simulations (Fig. 3).

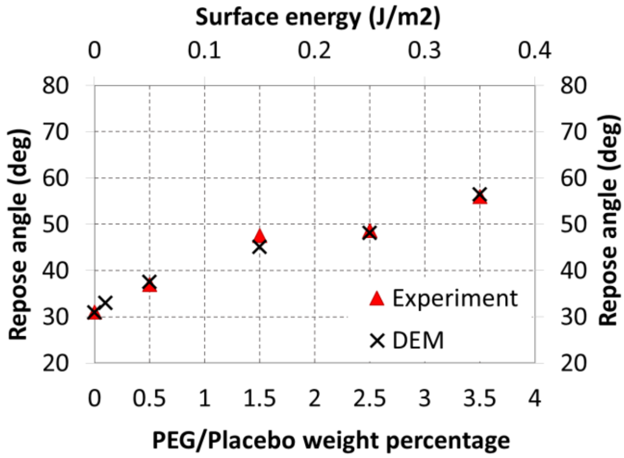

Fig. 3 : Calibration of particles surface energy versus their levels of coating using the angle of repose.

3. Results

Once all the particles are characterised and the surface energy of the coated placebo granules is calibrated, particles are mixed (Table 1) and introduced into the test box (Fig. 1) to form the heap. In the first test, particles are uncoated, i.e. they are free flowing, so their surface energy is set equal to zero. In this situation, although enzyme placebo granules are rounded and relatively larger than BP, they accumulate in the central zone of the heap due to their higher density, which is observable from the front view of both experiment and DEM simulation (Fig. 4).

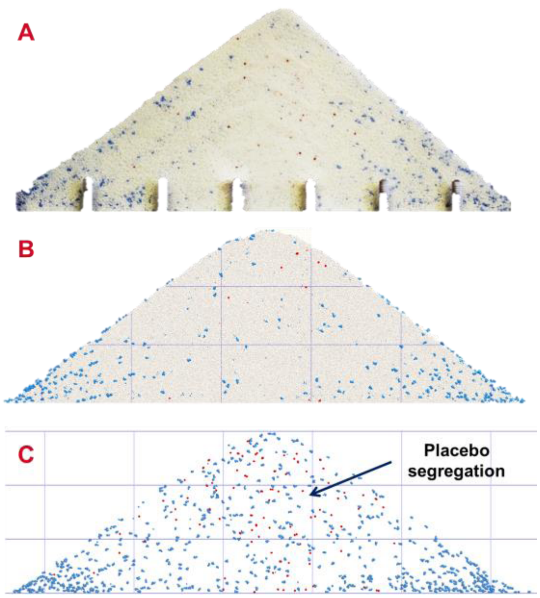

Fig. 4 : Heap formation of ternary mixture of BP (white), TAED (blue), and uncoated enzyme placebo (red) particles in A) experiment, B) DEM, and C) DEM-front thin layer when BP is removed.

In Fig. 4 (C) a thin layer from the front side of the heap (from DEM simulation) is displayed and the BP particles are removed to further analyse the mixture. This figure indicates the segregation of TAED particles in the corners of the heap and accumulation of the placebo granules in the centre which is in agreement with the experiment. Nevertheless, the experiment does not give a full picture of the mixture as the segregation pattern through the depth of the heap is not visible.

In the second test, the enzyme placebo granules are coated by 2.5 wt.% of PEG 400, mixed with BP and TAED and introduced into the test box to form the heap. Using the calibration study, shown in Fig. 3, and the cohesion number the equivalent interfacial surface energy values for placebo-BP, placebo-TAED, and placebo-placebo are predicted to be 0.037, 0.06, and 0.25 Jm^{-2}, respectively.

It is observed from Fig. 5 that the coated enzyme placebo particles do not accumulate in the centre anymore and the particles are distributed all over the heap leading to less segregation. Nonetheless, the distribution pattern of TAED particles is still the same as before meaning that the coated minor ingredients in the mixture has not affected the general behaviour and flowability of the mixture. This is also understood from the very similar repose angles of the uncoated (36°) and coated (37.6°) systems showing a negligible reduction in the mixture flowability after the coating.

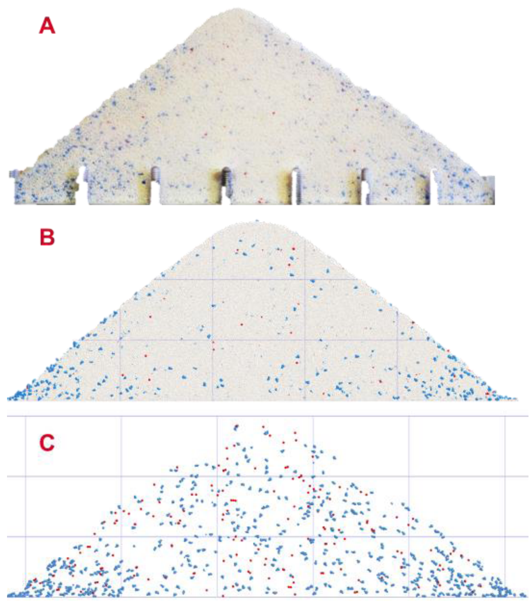

Fig. 5 : Heap formation of ternary mixture of BP, TAED, and coated enzyme placebo particles in A) experiment, B) DEM, and C) DEM-front thin layer when BP is removed.

To analyse the segregation quantitatively, the whole heap is divided into 21 bins including 7, 3, and 1 sections in width, height, and depth of the heap, respectively, as shown in Fig. 6. The Coefficient of Variations (COV) of the TAED and enzyme placebo particles are calculated based on their mass concentrations in each bin. It is observed that the COV of TAED particles is 0.76 for uncoated and 0.74 for coated systems which are very close. This result was expected as the coating has been done only on the enzyme placebo granules and the

DOI: 10.1051/epjconf/201714006024

mixing pattern of the entire system is not affected by coating the minor components, i.e. enzyme placebo granules. On the other hand, a significant enhancement in distribution pattern of the enzyme placebo granules is observed after coating. The COV of the placebo granules before coating was 0.46, while it is reduced to 0.29 after coating, i.e. nearly 37% reduction in segregation index.

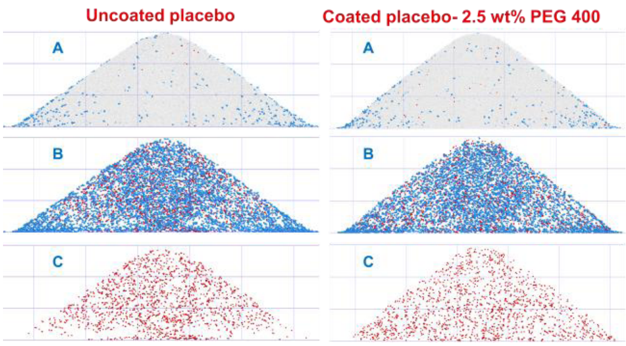

Fig. 6. Particles distribution before and after coating. Figure (A) the full image of the heap from the front, (B) the heap displaying TEAD and enzyme placebo particles, and (C) the heap displaying the distribution of enzyme placebo.

4. Conclusion

The segregation tendency of a ternary mixture of particles differing in shape, size, and density has been analysed for the case in which one component, being present as a minor content, readily segregates. To mitigate the extent of segregation this component has been made sticky by coating with a thin liquid layer before mixing with the other components. As a model system, the main ingredients of home washing powder (i.e. BP, TAED, and enzyme granules, the latter in placebo form) have been used and the segregation during the heap formation has been measured experimentally and analysed by numerical simulation using DEM. It is observed that uncoated enzyme placebo particles (as the minor component) segregate in the central area of the heap due to their high density; whereas, the coated particles are well distributed through the heap with 37% reduction in COV. At the same time, TAED particles segregate in the corners of the heap mainly because of their large size compared to the BP particles. It is observed that the distribution pattern of TAED does not change after coating of the enzyme placebos. Furthermore, comparing the repose angles of the mixture before and after coating shows a negligible reduction in flowability of the mixture after coating. These trends can be readily predicted by numerical simulation by DEM taking account of measured particle properties such as shape, density, size, and adhesion.

The authors would like to thank the Advanced Manufacturing Supply Chain Initiative (AMSCI) for their financial support. In addition, we would like to thank Claire Duckitt (Procter and Gamble) for project coordination.

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