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An experimental and numerical study of packing, compression, and caking behaviour of detergent powders

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ABSTRACT

This paper presents an experimental and numerical study of the packing, compression, and caking behaviour of spray dried detergent (SDD) powders with a two-fold aim: an experimental process of observation and evaluation of the packing, compression and caking behaviour of SDD powders, and a numerical approach based on discrete element modelling (DEM). The mechanical properties, including the stress–strain response and the corresponding porosity change as a function of consolidation stress in a confined cylinder, the stress–strain response during unconfined shearing and the cake strength as a function of consolidation stress, were evaluated and compared for different SDD powders using an extended uniaxial tester (Edinburgh Powder Tester – EPT). The experiments using EPT showed excellent reproducibility in the measurement of packing, compression and caking behaviour and were therefore very useful for describing the handling characteristics of these powdered products including screening new products and different formulations. It was found that the sample with higher moisture had lower bulk porosity but higher compressibility and cake strength. The porosity, compressibility and cake strength were found to vary across different size fractions of the same sample. The larger sieve-cut samples had higher initial bulk porosity, compressibility and cake strength. It is revealed that moisture plays a significant role in packing, compression, and shearing behaviour of the powder. Three-dimensional DEM modelling using a recently developed elasto-plastic adhesive-frictional contact model showed that the contact model is able to capture the detergent behaviour reasonably well and can be used to model complex processes involving these powders.

1. Introduction

Powder packing, compressibility, and flowability are important measures for industrial particulate solids, such as household and personal care products, chemicals, fertilizers, coal, cements, explosives, dyes and pigments. The packing behaviour of a powder in a container is determined by its initial microstructure and the ensuing mechanical processes including compression, shear, vibration and impact, which occur during transportation, for example. For the manufacturing of particulate detergents, bulk porosity is an important variable to control since most consumer doses are measured by volume and the solubility of detergent powders normally increase with increasing porosity. In addition, the compressibility of powders can influence their appearance and volume in containers once they reach consumers. Caking is a phenomenon where free flowing powders are transformed into lumps, aggregates or eventually into a coherent mass. Caking of powder can have adverse effects on solubility, mixing, and dispersion resulting in loss of products, delays in launch and consumer complaints. It can also cause storage and handling related problems including hopper/bin arching and ratholing, resulting in no flow. According to an estimate by Griffith (1991), the cost of unproductive cake products was in an excess of 1 billion USD in the USA alone in 1985.

The packing of porous powder is governed by inter-particle and intra-particle porosity. Several factors including particle shape, absolute size, size distribution, and surface properties (stiffness, friction, and adhesion), affect inter-particle porosity. In addition to particle properties inter-particle porosity may also depend on size, shape, and roughness of the container as well as the method and intensity of deposition (Yu, 1989). It is generally accepted that deviation of particle shape from sphere tends to increase the inter-particle porosity of mono-sized particles (Yu & Standish, 1993). Porosity is found to be independent of particle size for particle sizes above 100 μm (Yang, Zou, & Yu, 2000). For particle

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Nomenclature

C_u	coefficient of uniformity
D_{60}	diameter of particle at 60% passing (m)
D_{10}	diameter of particle at 10% passing (m)
e	co-efficient of restitution
f_0	constant adhesion (N)
f_n	contact normal force (N)
f_t	contact tangential force (N)
f_{ct}	coulomb limiting tangential force (N)
f_{nd}	normal damping force (N)
f_{ts}	tangential spring force (N)
f_{td}	tangential damping force (N)
f_{hys}	hysteretic spring force (N)
$f_{ts(n-1)}$	tangential spring force at previous time step (N)
k_1	loading stiffness parameter (N/m)
k_2	unloading/reloading stiffness parameter (N/m)
k_{adh}	adhesive stiffness parameter (N/m)
k_t	tangential stiffness (N/m)
m^*	equivalent mass of the particles (kg)
n	non-linear index parameter
η_{inter}	inter particle porosity
η_{intra}	intra particle porosity
η_p	particle porosity
R_i	distance from the contact point to the particle centre of mass (m)
v_n	relative normal velocity (m/s)
v_{pores}	specific volume of mercury penetrating the particle pores (L/kg)
v_t	relative tangential velocity (m/s)
w	moisture content (%)
β_n	normal dashpot co-efficient
β_t	tangential dashpot coefficient
Φ	angle of shearing resistance (°)
Δf_{ts}	Incremental tangential force (N)
δ	normal overlap (m)
δ_{max}	maximum normal overlap (m)
δ_p	plastic overlap (m)
ρ_s	skeletal density or particle density (kg/m^3)
ρ_b	bulk density (kg/m^3)
η	sample bulk porosity
μ	co-efficient of friction
μ_r	coefficient of rolling friction
τ_i	total applied torque (N m)
ω_i	unit angular velocity vector (radian/s)

diameters smaller than 100 μm, the ratio of inter-particle force to the weight of particles can be greater than unity (Krupp, 1967), resulting in different packing behaviour. Higher inter-particle force ratios cause formation of chain-like structure leading to high porosity (Yang et al., 2000). For cohesionless powders, as the spread of the particle size distribution (PSD) increases, the porosity decreases because the smaller particles fill the pores between larger particles. The effect of PSD on porosity of cohesive material is not very well understood and is influenced by the complex adhesive forces that exist. In addition, the intra-particle porosity of a powder may depend on chemical composition, and shrinkage or puffing effect due to drying (Hecht & King, 2000a, 2000b).

The powder compressibility may result from particle rearrangement, breakage of loosely bonded agglomerates into primary particles, failure of the particle during elasto-plastic deformation, and fragmentation of the primary particles (Heckel, 1961; Hersey & Rees, 1970). These mechanisms do not happen in sequence and usually overlap each other (Hersey & Rees, 1970). For agglomerated cohesive powders subjected to increasing consolidation stress, particles are likely to undergo rearrangement and loosely bonded agglomerate may break without excessive deformation at the particle contacts. The rearrangement of the particle will depend on the particle shape (Cho, Dodds, & Santamarina, 2006; Güden, Celik, Hizal, Altindiş, & Cetiner, 2008), size and size distribution (Hersey & Rees, 1970), rolling and static friction (Sheng, Lawrence, Briscoe, & Thornton, 2004), and adhesion (Mehrotra, Chaudhuri, Faqih, Tomassone, & Muzzio, 2009). The breakage of an agglomerate will also depend on bond strength. As the consolidation stress is increased, elasto-plastic deformation of the particles leads to squashing and reduction in intra- and inter-particle porosity. On further application of stress, fragmentation of the primary particle may occur and excessive deformation may lead to work hardening.

The cake strength of powder at an applied consolidation stress is affected by particle size, size distribution, friction, shape, humidity, moisture content, plastic deformation and adhesion at the particle contact etc. Several experiments including shear cells (Jenike, annular, and Peschl), tensile test, creep test, penetration test, caking index test, blow test, and uniaxial test have been used for the measurement of caking propensity (Cleaver, 2008). Each tester has its own advantages and disadvantages, which were explained by Schwedes (2003). Uniaxial test has widely been used to study the caking or shear behaviour of powders (Bell, Catalano, Zhong, Ooi, & Rotter, 2007; Enstad & Ose, 2003; Freeman & Fu, 2011; Parrella, Barletta, Boerefijn, & Poletto, 2008; Röck, Ostendorf, & Schwedes, 2006; Williams, Birks, & Bhattacharya, 1971; Zhong, Ooi, & Rotter, 2005) in industrial practice because of its simplicity and rapidity in conducting a test. Repeatability of measurement is one of the major concerns for uniaxial testers. An extended uniaxial tester, the Edinburgh Powder Tester (EPT), has been developed at the University of Edinburgh, with a focus on robustness, repeatability and speed for industrial solids measurement (Bell et al., 2007).

The discrete element method (DEM) has increasingly been used to model discrete phenomena including powder packing (Dong, Yang, Zou, & Yu, 2006; Yang et al., 2000; Yang, Zou, Dong, An, & Yu, 2007; Yen & Chaki, 1992), compaction (Morgeneyer et al., 2005; Redanz & Fleck, 2001; Samimi, Hassanpour, & Ghadiri, 2005; Sheng et al., 2004), and powder flow (Baxter, Abouchakra, Tüzün, & Mills Lamptey, 2000; David, García-rojo, Herrmann, & Luding, 2007; Luding et al., 2004; Mehrotra et al., 2009; Moreno-Atanasio, Antony, & Ghadiri, 2005). To date the DEM modelling of cohesive powders has been less successful in producing quantitative predictions.

The major objective of this paper is to study packing, compression, and caking behaviour of spray dried detergent powders using the EPT, and to model the full spectrum of the loading regimes from compression to shear failure using DEM. The EPT is used to measure the mechanical properties including the stress–strain response and the corresponding porosity change as a function of consolidation stress in a confined cylinder. In addition, the stress strain response during unconfined shearing and the cake strength as a function of consolidation stress is evaluated. The physical properties of the powders, which may affect the mechanical properties, are also measured. These include moisture content, particle size, size distribution, shape, inter- and intra-porosity. DEM modelling is then used to simulate the packing, compression and shear behaviour, which is compared with the experiments for one example detergent powder. The simulations utilised a recently developed contact model that uses hysteretic non-linear loading and unloading paths to model the elasto-plastic permanent contact deformation and an adhesion parameter which is a function of the maximum contact overlap (Thakur, Morrissey, Sun, Chen, & Ooi, 2011).