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Numerical analysis of density-induced segregation during die filling

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ABSTRACT

In this study, segregation behaviour of binary granular mixtures with the same particle size but different densities during die filling in the presence of air was investigated using a combined discrete element method (DEM) and computational fluid dynamics (CFD) approach, in which the kinematics of particles was modelled using DEM, the motion of air was analysed using CFD and a two-way coupling of the particles and the air was incorporated. The depositions of powder from stationary and moving shoes into the die cavities of different geometries were simulated and the corresponding segregation behaviours were analysed. It has been found that, for die filling from a stationary shoe, the concentration distributions of the heavy and light particles along the die width mainly depend on the initial spatial distribution of the granular mixture in the shoe. For die filling from a moving shoe, a low concentration of light particles on the leading side of the die (referring to the direction of the shoe motion) is observed for die filling with a square die, in which the process is dominated by nose flow. The density difference can cause segregation along the die depth with a low concentration of light particles at the bottom. The presence of air enhances this segregation tendency by resisting the flow of light particles into the bottom of the die and causes a higher concentration of the light particles at the top. Finally, the segregation index, defined as the volume weighted root-mean-square deviation in the content of light particles, was introduced to quantify the degree of segregation in the horizontal and vertical directions. It has been found that the degree of segregation is determined by the presence of air and also the powder flow pattern.

1. Introduction

Segregation is a phenomenon in which a homogeneous mixture of particles with different physical properties (particle size, density, shape etc.) becomes spatially non-uniform in such a way that particles having the same property congregate in one part of the mixture [1]. Segregation detrimentally affects the content uniformity and mechanical properties of products manufactured in a number of powder handling industries, such as powder metallurgy, ceramic, pharmaceuticals, mineral processing and food industries. Therefore, understanding segregation is crucial for improving the processing efficiency and product qualities in these industries.

Hence, extensive studies have been conducted to understand the segregation in various powder handling processes. For example, segregation during hopper flow was investigated by Ketterhagen et al. [2,3], who showed that the degree of segregation upon discharge was significantly influenced by the particle size ratio, hopper wall angle and particle–wall friction, while it was slightly affected by the particle density ratio, hopper dimensions and particle–particle friction. For vertically vibrated binary granular mixtures, it was shown from Monte Carlo simulations [4] that the large spherical particles segregated to the top of the granular mixture. However, Hong et al. [5] illustrated that a downward movement of large hard spheres could happen under some conditions, and they proposed a phase diagram for the upward/downward transition in terms of the particle size and mass ratios, based on the analysis of the competition between percolation and condensation. Two other criteria for the transition of upward/downward movements of large particles were developed by Jenkins and Yoon [6] based on a hydrodynamic theory and Trujillo et al. [7] based on the analysis of the competition between buoyancy and geometric forces, respectively. Density-induced segregation in vertically vibrated binary granular mixtures has also been investigated by Yang [8] and Shi et al. [9]. From DEM simulations, Yang [8] showed that the heavy particles tended to gather around the central region and the concentration of light particles was higher at the top compared to that of heavy ones. Shi et al. [9] observed a layer of light particles at the top of the powder bed in their experiments, and the thickness of this top layer depends on the density ratio. For chute flow, Khakhar et al. [10] found that density-induced segregation occurred with the heavier particles sinking to lower regions and the size-induced segregation was influenced by the particle inelasticity and inter-particle friction. When a mixture was poured to form a heap, the larger or lighter particles flowed down to the bottom of the free surface, whereas smaller or heavier particles sank into the heap close to the pouring point, as observed by Drahun and

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Bridgwater [11]. Olivieri et al. [12] experimentally investigated the segregation in a gas fluidized bed, and showed that the transient fluidization regime, which depended on the combination of particle size and density, dictated the segregation patterns.

Die filling is a general processing stage during the manufacture of particulate products in a number of industries, including pharmaceutical, powder metallurgy, ceramic and chemical industries, in which the powder blends generally consist of particles of different sizes and densities and air is normally present (i.e., production in a vacuum is a rare practice) [13–22]. It has been shown that the powder flow during die filling is complicated as it is determined by a number of factors [13–19], in particular, the powders interact with the air presence during the process in a sophisticated manner [14,15,18,19,22]. Consequently, segregation is more likely to occur if powder mixtures are employed as opposed to mixtures of larger grains. Segregation of binary mixtures during die filling was investigated by Lawrence and Beddow [20,21]. Their experimental results showed that size segregation occurred by a sifting mechanism whereby fine particles can filter down through the matrix of coarse ones, which results in a fines-rich region at the bottom of the die and a coarse-rich region in the periphery of the die cavity [20]. However, the difference in particle densities did not play a significant role in causing segregation in their experiments [20]. By using a vibrating die [21], the radial segregation was reduced due to the vibration, while the vertical segregation was found to depend on the amplitude and frequency of the vibration. When the die was oscillated at low or high amplitude, the powder mass was quiescent or bouncing and the vertical segregation was minimized; when the die was oscillated at intermediate amplitude and high frequency, the churning of powder mass occurred and the vertical segregation was increased.

Nevertheless, it is worthy to mention that the size of particles used by Lawrence and Beddow [20] for investigating the density-induced segregation was ca. 500 µm, for which the effect of air presence was negligible due to the relatively large particle size [22]. As the particle size becomes smaller (say less than 200 µm), the presence of air has a more significant impact on the flow behaviour of particles of relatively low densities [22]. Consequently, a better understanding of the segregation during die filling is awaiting. Therefore, the aim of this study is to examine the density-induced segregation during the die filling process and to investigate the effect of air on the segregation, for which a coupled DEM/CFD method is used and die fillings in air and in a vacuum are simulated.

2. Computational set-up

The coupled DEM/CFD method was originally developed by Kafui et al. [23] to model a two-phase (gas–solid and liquid–solid) flow. Using this method, a powder is modelled as an assembly of solid spherical particles which interact with each other and the interaction is determined with rigorous contact models based upon classical contact mechanics [24,25]. The position of each particle within the system is incremented at fixed time steps by integrating the equations of motion according to Newton's second law. The air is treated as a continuous fluid phase governed by the continuity and momentum equations. A fluid–particle interaction scheme is introduced to model the two-way coupling between the two phases. A detailed description of the DEM/CFD method is provided in [23].

All simulations reported are two dimensional (2D). In the 2D model, the centres of particles distribute in the same plane and the displacement perpendicular to the plane is prohibited. Therefore, caution should be taken when extrapolating the results from 2D systems to the 3D systems for which the third dimension is crucial to the powder flow, mixing and segregation behaviours [2]. In this study, the binary mixture bed is treated as a monolayer of spheres, from which the void fraction is calculated with the particle diameter as the thickness of the bed. The schematic layout of the die filling system with a stationary shoe is shown in Fig. 1a. The system is composed of a top

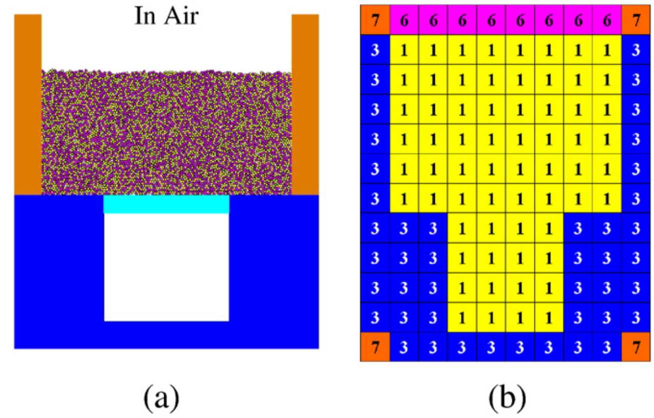

Fig. 1. (a) Computational set-up for die filling from a stationary shoe with a square die cavity and (b) a schematic diagram of the computational fluid cells and boundary conditions [1: interior fluid cell; 3: impermeable wall, no slip boundaries; 6: continuous gas outflow wall cell, free slip; 7: corner cell].

container that is generally referred to as a shoe, a bottom container (i.e., a die) and a shutter at the top of die, which is used to hold the mixture in the shoe before die filling. Initially, a well-mixed binary mixture is randomly generated as a granular gas (no contacts) in the shoe. The mixture consists of spherical particles of an identical diameter of 130 µm but different densities. The light and heavy particles are assumed to have densities of 2100 kg/m^3 and 7800 kg/m^3 and are colour-coded in yellow and magenta respectively for visualisation purposes. After generation, with the die opening closed by the shutter, the particles are deposited in the shoe under gravity until reaching a static state (i.e. the velocities of particles are of the order of 1 µm/s). The die filling is started by instantaneously removing the shutter and the powder then flows into the die from the shoe under gravity. The particles are assumed to be elastic with a Young's modulus of 8.7 GPa, Poisson's ratio of 0.3 and both inter-particle and particle–wall friction are set to a value of 0.3. The width of the shoe is 14 mm

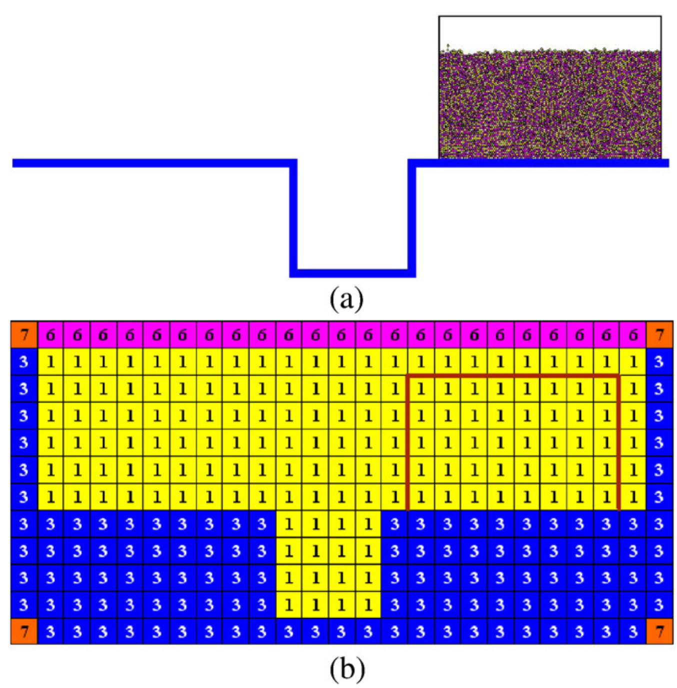

Fig. 2. (a) Computational set-up for die filling from a moving shoe with a square die cavity and (b) a schematic diagram of the computational fluid cells and boundary conditions [1: interior fluid cell; 3: impermeable wall, no slip boundaries; 6: continuous gas outflow wall cell, free slip; 7: corner cell].