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Segregation in the tank of a rotary tablet press machine using experimental and discrete element methods

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ABSTRACT

The segregation phenomena is one of the most important problems in tablet press machines, as it can induce an incorrect composition of the tablets and, thereby, modify its mechanical or physical properties. For that reason, the purpose of this work is to analyze the segregation of a binary mixture that is produced in the tank of a prototype of a rotary tablet press machine with gravity feeder using the discrete element method (DEM). For that purpose, a DEM simulation model was used to identify the mechanisms of segregation in several tanks of differing shapes with two widths and various filling and feeding methods. Thus, it was possible to determine that the segregation index (SI) that was obtained in the Short design was the lowest, regardless of the width of the tank or the method of feeding that was used. Moreover, by analyzing the effect of the width and the method of feeding the tanks, it can be concluded that it is possible to predict the segregation that is created in the prototype of a rotary tablet press machine with gravity feeder by a simplified simulation model (in which a narrow tank is filled once) that reduces the simulation time by 95%.

1. Introduction

Segregation is a phenomenon in which a homogenous mixture of granular materials of differing properties (size, density, shape, etc.) tends to be heterogeneous. This phenomenon is one of the most important problems in many industries that use granular materials in their processes, including the pharmaceutical industry, the food industry, the mineral industry, the powder metallurgical industry, etc. For that reason, it is important to know how the mixtures behave in the different processes. However, it is usually difficult to analyze the behavior of a mixture by an experimental procedure. Consequently, mathematical models are normally used to predict the behavior. The Discrete Element Method (DEM) that Cundall and Strack proposed [1] is a numerical method that permits the simulation of the motion of a granular material as separate particles (discrete elements).

The use of DEM simulations has been extended to a wide variety of processes in recent years due to the evolution of computers. DEM simulations have been used to study the evolution of the mixtures in different blending machines in order to improve their designs [2–4], simulate the mill process [5,6], analyze the covering of the tablets [7], study the compact of a tablet [8,9], simulate the sintering process [10–12], etc.

The study of segregation is particularly important for the tablet press machines that are used in industries such as the pharmaceutical and food industries. The mass variations or deviations in the proportion of materials in a tablet can result in poor tablet quality or health problems for those who consume them [13]. The effects of the particle size or size distribution on the uniformity of the content has been studied to ensure conformity to the United States Pharmacopeia Standard [14,15].

There have been many studies of segregation in various devices. Because of the similarity of the latter to the main parts of this type of machine, these studies can serve as references in studying the segregation that the tablet press machines create.

The segregation that is created while the hopper is filled and discharged has been studied by several authors [16–25]. These processes have been analyzed experimentally, using DEM simulations or continuum models. The methods have been used to predict the segregations of the material [16–21] or the flow patterns of the discharge [19,22–25]. In all of these works, the hopper is emptied by gravity or using a belt conveyor at the outlet. This last mode causes the flow patterns of discharge to resemble the patterns that are produced when a die moves under the hopper.

Related to the filling die process are several studies of the weight of material that is contained in the dies [26], the segregation (by size or density) that is created during the dies filling [27–30] or the fluidity of the materials [31,32]. In all of these cases, the system consists of a hopper and a die. In some cases, the die and hopper remain at rest [27–29]. Alternatively, the die moves below a stationary hopper [30] or the hopper moves over a stationary die [27–29,31]. The mobile part

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moves linearly in all of these cases, whereas the dies in a rotary tablet press machine follow a circular path.

The behavior of the material that is used in rotary tablet press machines with a feed frame has been studied by several authors experimentally [33–35] and by simulation [36–39]. In these studies, the influence of the process conditions on the residence time, the flow patterns or the attrition of the particles in the feed frame is investigated. Only [36] analyzed the size distribution of the particles inside the feed frame and the die to determine the particle size segregation that is produced by the adoption of different operating parameters. All of these studies concentrated on the influence of the feed frame design on the behavior of the material. However, the rotary tablet press machine that is analyzed in this research uses a gravity feeder, instead of a feed frame.

Gopireddy [40] simulated the operation of a rotary tablet press lab-scale gravity feeder. That study involved a set of mono-sized particles to analyze the influence of the velocity of the die disc, the size of the dies or the material properties on the mass deviations in the dies. However, the segregation was not studied because the granular medium consisted of particles of equal size.

In this study, DEM simulations are used to study the segregation that is produced inside the tank of a prototype of a rotary tablet press machine with gravity feeder during its filling and operation. Accordingly, the operation of the prototype was simulated and experimental tests were conducted. Three tank designs and three binary mixtures that consist of distinct proportions of two different sized granular materials were used. Some of the differences between the prototype used in this work and the conventional machines were the tank design, the prototype operation and the materials that were used. The tank designs were simple in order to permit an easier DEM model adjustment and validation. Moreover, the die disc of the prototype moved intermittently in order to enable the material that is contained in each die to be collected. However, this element moves continuously in conventional machines. The materials that were used in this work also differ from the powder or granules that are used in food or pharmaceutical industries to reduce the computational cost. The DEM model was validated by an iterative process in which the segregation results that were obtained by simulation and the experimental data were compared. After this validation, it should be possible to use this simulation model to analyze machines with geometries, operating conditions and material that are used conventionally in the industries in future works (by introducing the relevant modifications). Finally, this research investigated the possibility of analyzing the segregation by simplified simulations to reduce the temporal cost of examining a more complex system.

2. Materials and methods

This section presents the details of the equipment and materials that were used in this work, the characteristics of the DEM model, the methodology and the calculations that were made for a comparison of the results.

2.1. Tablet press machine used

A prototype of a single punch rotary tablet press machine with gravity feeder was used to provide experimental data. This prototype, which is shown in Fig. 1(a), was made of transparent polycarbonate. This material makes the visual analysis of the process easier, as it makes it possible to examine the material in the machine [22,23,41].

Fig. 1(b) shows the main parts of the machine. The prototype that was used consists of a fixed tank (1), a hopper (2) that is used to fill that tank and a mobile die disc (3) that has 20 dies (4) and rotates on a shaft (5). Three horizontal plates (6, 7 and 8) provide support for the die disc and prevent the material that the dies contain from falling. This prototype does not have the lower punches that compress the powder on the real single punch rotary machines, because the compaction process was not analyzed in this study. Two video cameras that are located in front of (9) and under (10) the prototype record the frontal view and bottom view of the tank, respectively. Also, a capacitive sensor (11) detects the presence of the dies (cavities in the die disc) and counts by digital counter (12) the number of the die that is being filled.

The machine's operation is based on the die disc rotation that permits the dies to move under the tank and to fill by gravity with the material that the tank contains. When a die crosses one of the tank's side walls, the granular material falls into the die and begins to fill it. The die is completely full when it crosses the opposite side wall. From that moment on, the contents of the dies remain confined between the horizontal plates. Finally, the material is collected at the extreme end of the plates.

The die disc has a height of 22 mm and a diameter of 420 mm. It has 20 dies that are cylindrical through-holes with a diameter of 20 mm. The distance between each die and the center of the die disc is 150 mm. The tank is configurable. Thus, it can assume different lengths (L), widths (W) and slopes of the side walls (θ1 and θ2) (see Fig. 2(a)). As one can see, all of the possible configurations are simple (only polyhedral geometries can be obtained). This makes the tanks that are used in this work differ from conventional ones. Nevertheless, this fact makes the DEM model adjustment and validation easy. Three tank designs, named 'Short', 'Long' and 'Inclined' were used to determine how the length (L) and the slope of the side walls (θ1 and θ2) affect the segregation mechanisms and the discharge flow patterns. Two types of tanks were used in this study. Firstly, several tanks with a capacity that is similar to that of a conventional tank were used. The width (W) of these tanks, named '3D tanks', was 51 mm. Secondly, narrower tanks that were 20 mm in width and named '2D tanks' were used to simplify the analysis of the segregation mechanisms and to reduce the simulation time [17,18,23]. A total of six configurations were used in this study (see Fig. 2(b)). The hopper that was used to fill the tank is funnel-shaped. Its side walls form an angle of 67° with the horizontal direction. The dimensions of the hopper are shown in Fig. 2(c).

2.2. Materials

A binary mixture of two different sized granular materials was used in this study. Both materials were wheat semolina and had a similar density and a substantially spherical shape. Their diameter ratio was 2:1 (see Fig. 3(a)). Image processing techniques and statistical analysis were used to calculate the mean equivalent diameters. The densities of the particles were determined by a pycnometer, according to the ASTM D 854-14 standard. The dimensions and mean densities of the particles are shown in Table 1. The diameters of these particles were much greater than that of the materials that are normally used in the pharmaceutical industry, but similar to that of the particles that are used in the food industry for the compaction of food additives. These large particles were selected for the experiments in order to calibrate the simulations with the same materials used in both cases. This reduces the computational cost. The fine particles were colored to distinguish the materials, as other authors had done [2,22,23]. Three different mixtures were used. The first consisted of fine material and coarse material in proportions of 25% and 75% (by weight), respectively. The second consisted of each material in proportions of 50%. The third consisted of fine material and coarse material in proportions of 75% and 25%, respectively. The three mixtures are termed '25f-75C', '50f-50C' and '75f-25C' hereafter.

2.3. Tank filling methods

In this study, two different tank filling methods were used [16,17]. These methods were layered filling and industrial filling. In layered