Discrete Element Method Simulation of Filling Level in Planetary Ball Mill

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Abstract: - In this study, DEM (discrete element method) was used to improve our understanding of the fundamental processes involved in the ball milling process, with a particular emphasis on the effect of the many different filling levels in planetary ball mills. This DEM methodology facilitates the simulation of the behavior of balls and powder particles inside the vials, enabling an understanding of the nature of the material milling and the structure of the flow. The major benefit of the DEM technique is the ability to incorporate interrelationships among different milling parameters. The simulations indicate that changing the filling level has a significant effect on the ball milling process.

Key-Words: - planetary ball mill, simulation, discrete element method, modeling, filling level, milling parameters.

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1 Introduction

Planetary ball mills have emerged as a tool, in materials science, for efficiently breaking down a wide variety of materials. These high-energy mills are used in working with very sensitive powder applications e.g. pharmaceuticals and fine chemicals to nanomaterials, where the purity and stability of the material are of vital importance. As the vials used in this work have a larger size than the common scale used, such one is able to be inserted into a planetary ball mill for milling that is rotated with respect to their own axes, and simultaneously around the central axis in opposite directions. This provides a relatively complex centrifugal pseudo-acceleration, which in turn impacts the movements and collisions with the milling media inside of the vials. In order to obtain the intrinsic mechanisms involved in planetary ball milling, researchers used the Discrete Element Method (DEM) simulations. Through these simulations, valuable insights regarding the velocity distributions of particles, the character of the applied stress conditions, as well as the on overall filling level inside milling vials have been obtained, [1].

DEM has been used to model planetary ball mills which have not only shed light on particle dynamics but also offered the facility of choosing the right milling condition for targeted material properties. DEM, by simulating motion and interaction of milling media, can thus help researchers understand how the operational variables (rotational speed, vial geometry, and media size) control the milling process. Therefore, predictive models were designed to predict results including particle size distribution, milling efficiency, and material breakage type. In addition, DEM simulations have been used to investigate how the wear rate for both media and milling vials is affected by milling media material and shape, giving rise to more wear-resistant and efficient designs. These are essential properties to scale up laboratory results in industrial applications and for consistency in product quality and process efficiency. With the promises held by these simulation techniques in tuning milling processes for peculiar material needs, including novel nanomaterials production, fine-tuning of pharmaceutical powders, and development of new chemical compounds.

The Discrete Element Method (DEM) represents a numerical method often adopted in the modeling and optimization of ball mills, [2]. DEM relies on computational techniques to analyze particle movement and collisions based on Newton's laws of motion. In previous research, [3], [4], we used DEM modeling to analyze the simulations of a planetary ball mill. The simulation of varying ball mills is a significant area of research utilizing DEM in numerous studies. The authors of the study [5] revealed that the impact energy of the balls greatly affected the effectiveness of the milling process. During the comparative analysis in [6], steel balls and alumina balls were evaluated for their effectiveness in grinding the cement clinker using a population balance model (PBM) and DEM, which concluded that energy savings of up to thirty-five percent could be achieved in milling when alumina balls were used to replace steel balls. In addition to the aforementioned considerations, a computational fluid dynamics (CFD) analysis was conducted to examine the influence of milling circumstances on the particle size, [7]. In [8], it was used DEM simulations to study the thermal transfer properties of the ball-milling components. They found that the simulations corresponded to an experimental investigation, thereby validating that the simulations represented a realistic approximation of the phenomena being modeled. Similarly, the study [9] used a DEM approach to simulate ball motion in planetary ball mills. A strong correlation between the experimental and simulation results was found across different test conditions. Separately, the study [10] compared the results of simulating the charging behaviour in a centrifugal grinding device to their experimental results. The simulation results were also found to correspond closely with the experimental data. In [11], it was used DEM simulations to investigate the mechanisms responsible for high-energy planetary ball milling processes. These results lead to the conclusion that using DEM simulation can enhance our understanding of how operational variables affect the dynamics of the system. Additionally, the study [12] developed a new technique to model DEM balls in considering slurry within a tumbling mill. The simulations indicated that specific impact energy directly correlated with the milling rate within the sample material. Furthermore, the authors suggested that the energy input was an important variable within the milling process. The study [13] developed a new mechanistic Universidade Federal do Rio de Janeiro (UFRJ) mill to model particle size distribution using a dry laboratory planetary mill. Their simulations indicated that the proposed model gave accurate predictions for the model. The study [14] presented a new method that models the three-dimensional profile of an end-milled floor surface using various variables including tool setting error, tool workpiece vibration, tool path overlap, and cutting motion. The results demonstrated good agreement between observed and predicted three-dimensional topography.

The primary purpose of this study is to achieve a better understanding of the phenomena occurring during rotating dynamics in a laboratory-scale planetary ball mill through DEM simulations at different fill levels.

2 Used Equipment

Planetary ball milling is a commonly used technology in materials science and engineering, primarily in the production of advanced materials and the size reduction of powders. The technique utilizes the rotation of a grinding vial around its own axes simultaneously with the turntable (or sun wheel) spinning in the opposite direction, creating a complex dynamic motion. The combination of dual rotation creates a high-energy environment to which impact and shear forces are applied to the milling media which maximizes particle size reduction, mixing, and mechanical alloying, making planetary ball milling a staple method in the development of nanomaterials and fine powder processing.

The milling capacity of a planetary ball mill is a result of several interactions of important mechanisms. First, it relies on the impact force generated as the milling media strikes the material being milled, resulting in fracture and size reduction of the milled material. Shear force is also important, which occurs when particles become entrapped between colliding balls or between the balls and the vial walls. This force is important to facilitate the plastic deformation of particles, re-shaping the workability of the particles, and blending the milled material. Impact and shear forces can result in not only a reduced particle size but also play a vital role in solid-state reactions, phase changes, or in some cases the formation of amorphous phases, which is a key step in the synthesis of new materials. Moreover, the intense localized energy dissipation within vials contributes to the activation of chemical reactions, enabling the formation of new compounds and alloys that might be challenging to achieve using conventional methods.

The energy transfer in a planetary ball mill is significant and is characterized by the high kinetic energy imparted to the powder by the colliding milling media. However, accurately quantifying the energy transferred during milling is challenging because of the intricate nature of the milling process, which involves variable factors, such as milling speed, media size, and milling duration.

In this study, a high-energy planetary ball mill (manufactured by Fritsch, model Pulverisette 7, Germany) was employed, which is equipped with two vials that rotate around a single axis while the turn disc rotates in the opposite direction (Figure 1). Steel balls 15 mm in diameter were used as milling media. The planetary motion is simulated through a rotary motion of the vial around its axis, accompanied by the introduction of a rotating centrifugal pseudo-acceleration affecting the particles.

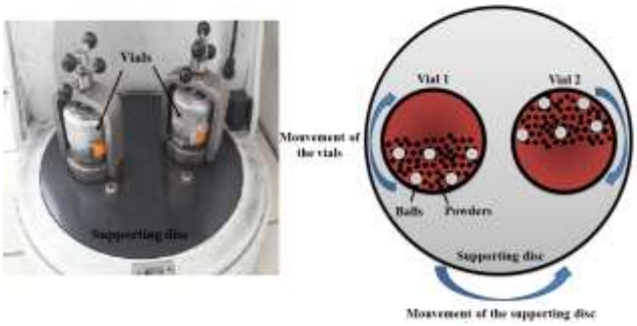

Fig. 1: a) P7-planetary ball mill apparatus, b) Schematic depicting the motion of the ball inside the vials

3 Simulation Procedure

The DEM simulations were conducted utilizing the commercially available EDEM 2021 software [15], which assumes that the particles are spheres and that minor overlap occurs during collisions. The model that has been employed in the analysis of the collision between two particles is predicated upon the linear spring-dashpot contact model, [16]. Figure 2 provides an overview of the configuration of the "Particle Shape Editor", which includes a number of commands (shapes, 3D model, properties, the format of template, etc). The following section outlines the steps required to create and organize an EDEM Material Model database. The following steps are required to create an EDEM material model database:

- Creating material categories
- Creating equipment materials
- Creating a bulk material and assigning shapes
- Defining material size distribution
- Defining the material interactions
- Saving an EDEM material model database
- Using EDEM material models in simulation

The use of CAD templates is useful for creating multi-spherical shapes.

In addition to the usual approaches for creating the EDEM material model database, careful calibration and validation were conducted on the simulation parameters to accurately replicate the actual milling process behavior. This involved modifying the input parameters (e.g. particle density, friction coefficients, and restitution) to match experimental data acquired from physical milling operations. The iterative process is vital for refining the DEM model and predicting the particle dynamics and energy transfer in the planetary ball mill precisely. To assess the validity of the simulations, anticipated results were compared against empirical data from earlier literature (e.g. particle size distribution and milling performance). Moreover, it is fundamental to ensure that model particles' shapes and dimensions are appropriate representations of manufactured particles to generate simulation results that are reliable and reproducible both scientifically and practically. The importance of demonstrating this congruence of particle shape is amplified when accurately modeling particle interactions associated with a milling process. The development of multispherical shapes in Computer-Aided Design (CAD) templates results in a substantially more faithful representation of nonspherical shapes compared to simple spheres, which enhances the level of realism of the model. In the simulations, to mimic the planetary motion of the mill as effectively as possible, both the vial's rotation around its own axis and the turn disc's rotation in the opposite direction produce the centrifugal acceleration needed for accurate modeling. The abovementioned process has been enhanced and integrated in order to create a strong and viable method for evaluating the influence of the combination of specific mill parameters on the comminution mechanism, which will lead to a better understanding of the interactions occurring in planetary ball mills.

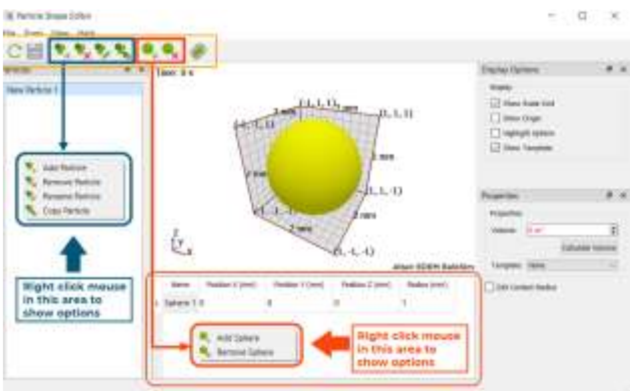

Fig. 2: The appearance of the particle shape editor.

4 Results and Discussion

The filling of milling media is an important parameter in characterizing particle wear and/or compression frequencies [17], and it determines milling quality [18]. In this work, we conducted simulations with varying media filling values of 40, 50, 60, and 70 percent. In the simulations, 25 mm diameter balls were employed, along with fine particle size distributions having a diameter of 3 mm.

Figure 3 illustrates the snapshots of DEM simulations, which demonstrate the impact of varying media filling values (40, 50, 60, and 70 %). The particles are colored in different colors based on their velocities as they are blue (lowest velocity) and red (highest velocity). As can be seen from the figure, the degree of mixing rises as the voids are filled, with segregation becoming a significant phenomenon at low filling levels. This phenomenon is due to the fact that there are not enough particles available to fill the cavities in the bottle, causing particles to trickle down into the ball charge, [19]. Similarly, the study [20] reported that the milling media concentration is directly proportional to the total filling level. According to the study [21], the motion of particles even changes from cataracts to cascading movement as the filling level increases from 10 to 30 %.

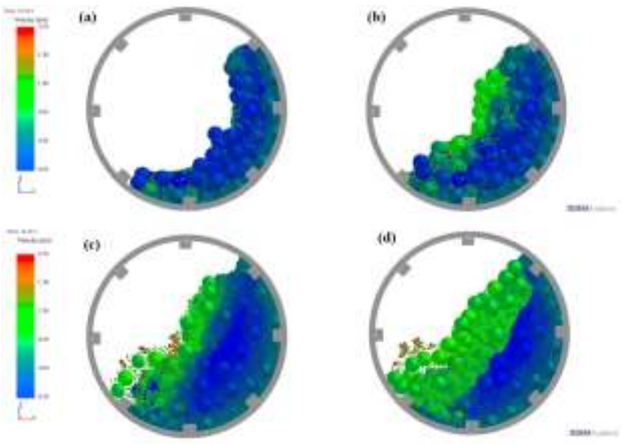

Fig. 3: Snapshots of DEM simulations showing different values of media filling:(a) 40 %, (b) 50 %, (c) 60 %, and (d) 70 %

A snapshot of the DEM simulation of the milling media at elevated milling speeds is shown in Figure 4. It can be observed that the acceleration of milling velocity results in an accumulation of particles in the vicinity of the vial's wall. Additionally, it can be seen that the particles are launched higher than the balls due to their higher mobility inside the vial. The results indicate a comparable pattern between the observed experimental and the simulated data.

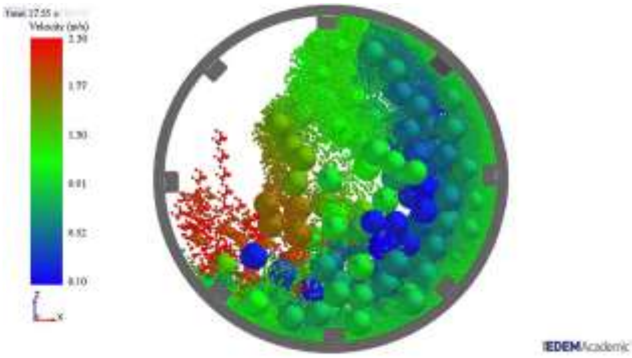

Fig. 4: Snapshot of DEM simulation of milling media at elevated milling speed

Increasing the milling speed may affect the particulate or ball movement within the vial. With this proposed model, it can clearly explain the phenomenon that occurred during the ball milling process.

The trends in particle behavior, as a function of the media filling level and the milling speed, provide further insight into optimizing the milling conditions for different material systems. As the media filling level is increased, the rate of particle-particle interactions and collisions increases, thus improving comminution efficiency and decreasing the risk of particle agglomeration. At higher filling levels, the free space available for particle motion becomes scarce, thus limiting their ability to move freely and decreasing the effective energy for milling particles. In contrast, at low filling levels, the available free space would lead to the free movement of particles, which can increase the chance of segregation and product inconsistency. The DEM simulations also illustrated that when the milling speed was increased, the net centrifugal forces acting on the particles were larger, resulting in higher particle velocities and faster mixing efficiency. Additionally, it would appear as conditions improved, the energy reached a chaotic state where added speed resulted in a greater discrepancy in velocities together with higher impact, higher kinetic energy transfer, and increased overall efficiency. Indeed, whilst this energy contribution led to improved performance in terms of rapid size reduction, it also increased the risk of early degradation of the milling media and vial. Conditions can be maintained in a positive and productive milling process once the disadvantages are controlled around process efficiency and product quality. These findings provide valuable insights into the important relationships between the filling level and milling speed that positively influence mill performance. It is particularly important to key strict attention to these relationships to ensure the desired material properties have been obtained in the processed material while reduced to a minimum where disruptions can disrupt the milling process efficiency.

5 Conclusion

In this research, a discrete element method (DEM) model was utilized for investigating the feed level in planetary ball mills, reporting a correlation between simulation results and experimental results. The results confirm the degree of filling is a key operational parameter related to the extent and degree of milling. Furthermore, it also shows that varying the milling speed has a real influence on the movement of the milling media (particles and balls) inside the vial. The DEM model that has been developed shows the capacity for describing much complexity with the ball milling processes and acts as a real advance for understanding what will happen as ball milling takes place. By exploring the effect of filling levels and milling speeds in a structured way, we have been able to provide unique insights into particle dynamics, energy transfer, and milling efficiency in general. These results highlight the significance of having improved operational parameters or variables in order to obtain the material properties that are intended, whilst limiting the less desirable consequences. The validated model thus serves as a powerful tool for enhancing the design and optimization of planetary ball milling processes, contributing to improved process efficiency and product quality.

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Declaration of Generative AI and AI-assisted Technologies in the Writing Process

During the preparation of this work the authors used Altair software in order to simulate filling level in a planetary ball mill. After using this tool/service, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

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Contribution of Individual Authors to the Creation of a Scientific Article (Ghostwriting Policy)

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Conflict of Interest

The authors declare that there are no conflicts of interest.