CHEMICAL ENGINEERING TRANSACTIONS
VOL. 114, 2024

A publication of AIDIC
The Italian Association
of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Petar S. Varbanov, Min Zeng, Yee Van Fan, Xuechao Wang
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ISBN 979-12-81206-12-0; **ISSN** 2283-9216

DOI: 10.3303/CET24114096

Discrete Element Method Optimization Simulation of Planetary Ball Mills Operating Conditions

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Planetary mills have garnered significant attention in various fields of material science, nanotechnology, and engineering due to their ability to finely grind and mix materials at the nanoscale. The study of such mills is often performed by using empirical approaches for the optimization of experimental conditions. Modeling is possible based on simple physics involving the interaction of DEM (Discrete Element Method) simulations, offering the possibility of studying planetary mills with a much deeper understanding of the process. This study focuses on the numerical characterization of planetary ball mills in terms of different parameters such as angular velocity, number of balls, and ball size. The influence of such parameters on the energy spectra of the mill is then found via DEM simulation, which is very useful information for modeling the breakage or adhesion processes inside a mill or scaling up such experimental mills to industrial processes. Results show that from all the useful power, 65.4 % and 54.0 % go into ball-wall shearing collisions for both 1 cm and 0.3 cm balls. At around 0.5 cm balls, there seems to be a minimum as only 46.7 % goes into ball-wall shear collisions. Despite this, those types of collisions take more power than any other for all the cases studied, being a ball size that is closer to the optimal value. This research, then, acts as a bridge between lab-scale conditions, which are easier and more cost-effective to optimize, and large-scale production, where optimization tends to be costly and difficult. The present study provides an understanding of the tools required to produce novel nanomaterials.

1. Introduction

The planetary ball mill has been attracting increasing attention in the laboratory field of mechanochemistry due to its advantages of high efficiency, small particle size achievable (i.e., nanoparticles), and low loss. The key to achieving excellent grinding products is adjusting the parameters of the planetary ball mill, including rotation speed, rotation direction, ball size, the filling ratio of samples and balls, running time, etc. (Nair et al., 2024). Generally, experimental studies are used to determine the optimal grinding conditions, but this approach is costly and time-consuming. Computer simulation is a helpful alternative to studying the complex physical phenomena in grinding. The Discrete Element Method (DEM) is a computational method used to simulate the behavior and the energy of particle systems, and it is suitable for simulating interactions and collisions between different media (Marchelli and Di Felice, 2021). Investigating the relationship between ground conditions and energy information of the planetary ball mill can provide design insights for industrial products. Some researchers have reported on the impact of energy at different grinding conditions by DEM. For instance, Hirosawa and Iwasaki (2021) explored the dependence of the dissipated energy of particles on the sizes and numbers of particles and balls using DEM in a planetary ball mill, and the results indicated that the particle-to-ball size ratio strongly affected the specific dissipated power rather than the ball-to-particle filling mass ratio. Jayasundara and Zhu (2022) analyzed the impact energy of the particles under different operating conditions, and the results showed that the impact energy was affected by the operating conditions of the mill and linked to the grinding rate for a given material. The research also reported that the correlation between impact energy

Paper Received: 25 April 2024; Revised: 9 September 2024; Accepted: 9 December 2024
Please cite this article as: Cabello R., Han J., Popescu A.E.P., Bonet-Ruiz J., Batlle G.C., Barreneche C., Dosta S., 2024, Discrete Element Method Optimization Simulation of Planetary Ball Mills Operating Conditions, Chemical Engineering Transactions, 114, 571-576 DOI:10.3303/CET24114096

and grinding rate followed first-order grinding kinetics, and mill performance decreased with increasing mill size. Ashrafizadeh and Ashrafizaadeh (2012) found that at certain rotational speeds, the kinematic and dissipated energy oscillate periodically in a planetary mill. Paramanantham et al. (2023) investigated the impact and contact behavior of the planetary ball mill to understand the movement of steel balls and iron particles inside the reactor vessel, and the DEM was used to understand the internal behavior of a planetary mill. Although many researchers have used DEM simulation to investigate the relationship between the energy and the operating conditions, to the best of our knowledge, there is relatively limited research on the shear energy and cumulative power in planetary ball mills. The shear energy plays a crucial role in planetary ball mills, affecting key performance indicators such as particle fragmentation and refinement, mixing homogeneity, as well as energy transfer, and dissipation. Reducing power consumption is not only beneficial for environmental protection and resource conservation but also enhances production efficiency and product quality, lowers production costs, and holds significant importance for the sustainable development of enterprises. Optimizing power consumption can be achieved by adjusting grinding conditions to alter both collision energy and shear energy in planetary ball milling. This enables more efficient operation of the planetary ball mill.

In this work, these properties, including the impact energy, the shear energy, the collision frequency, the power, and the cumulative power, are calculated for ball-ball and ball-wall under different simulation conditions using DEM. Firstly, the effect of the rotational speed in the planetary mill on the impact energy, the shear energy, the collision rate, and the cumulative power is investigated to analyze intrinsic relationships and establish optimal grinding conditions. Secondly, the effect of the ball size on the impact energy, the shear energy, the collision rate, and the cumulative power is investigated at 500 rpm in the planetary mill. Additionally, the cumulative power is also considered in different kinds of collisions.

2. Method

Simulations are performed with DEM commercial software Ansys Rocky DEM®. To perform the simulations, the movement and geometry of the mill must be carefully replicated. Planetary mills have two moving frames; they rotate around a central axis (sun wheel) and around the axis of the grinding container (planetary wheel) (Figure 1).

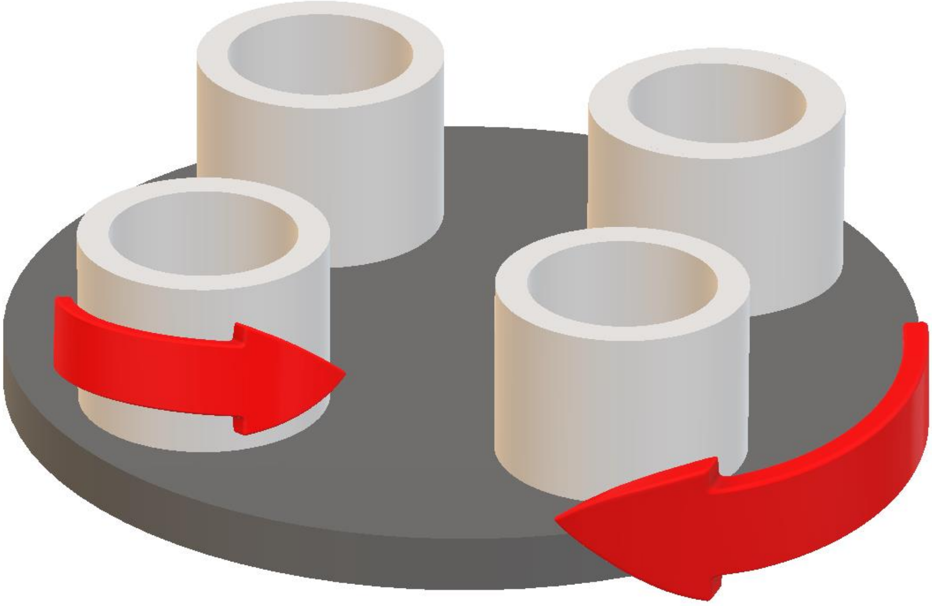

Figure 1. Rotation diagram of a planetary ball mill. Two axes of rotation are present: the vessels, in light grey, rotate along the central sun wheel axis, in dark grey, and around its own center of mass

The experimental apparatus that is to be simulated has the following operating conditions:

- The sun wheel rotating speed ranges from 0-290 rpm while the planetary wheel ranges from 0-580 rpm. The ratio at which the two wheels rotate is fixed and was measured via high-speed footage of the apparatus. The experimental apparatus often has a sun-top-planet rotation ratio of 2.
- The studied grinding balls have a diameter that ranges between 3 and 10 mm, are made of steel, and around 10-12 g of them are used in each grinding simulation. By fixing the amount of material, one of the

parameters of the mill that describes the volume occupied by the grinding balls is fixed, leaving one parameter less to optimize.

Only one of the four vessels present in the experimental setup is simulated, as each vessel has the same dimensions and is identical and situated symmetrically. The cylindrical vessel is 53 mm, both in height and diameter. It is meshed so that the curvature is well depicted when estimating collisions (Figure 2).

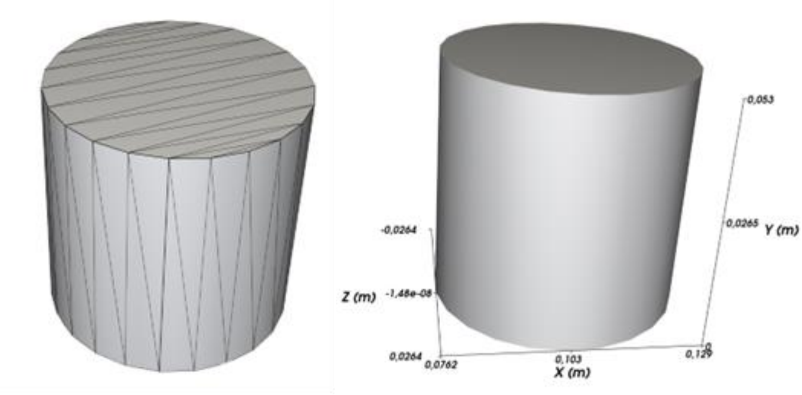

Figure 2: a) Mesh of the cylindrical vessel. b) Measurements taken in the program of the vessel

The tests change rotation speeds (100, 300, and 500 rpm) and ball diameter (3, 5, and 10 mm) and test all the different combinations between them. As the mass of material is the same in every simulation, there is a different number of balls depending on their size. All simulations are run for 10 seconds of operation, which is enough to stabilize the motion of the balls inside the mill and obtain steady energy results.

Table 1: Steel ball size and numbering for different diameters

Diameter (mm)	Total number of particles	Mass per particle (g)	Total mass (g)
3	93	0.11	10.23
5	20	0.511	10.22
10	3	4.08	12.24

The DEM simulation is based on Newton's second law of motion:

$$\sum F = m\frac{dv}{dt} \tag{1}$$

The normal contact equations are from the Hysteretic linear spring model based on the Walton-Braun theory (Walton and Braun, 1986). This model accounts for the plastic deformation of particles when the collision occurs. Additionally, the energy dissipation is not dependent on the relative velocities of neighboring particles, making the energy dissipation insensitive to other contacts (DEM Technical Manual, 2020). Tangential forces are estimated by using the linear Coulomb limit model, which linearly increases the force with respect to overlapping without exceeding Coulomb's limit, that is, the friction coefficient times the normal force (μF_n).

Collision statistics account for three different types of work: dissipation work, impact work, and shear work. Dissipation work is the amount of mechanical energy that is transformed irreversibly into other forms of energy. Impact work refers to the maximum amount of work transferred during a collision. It is the one that can lead to the breakage of particles, and it is defined as the integral during the loading stage of the collision of the normal contact force F_n over the overlapping distance s_n (Eq.2).

$$W_{imp} = \int_{loading} F_n \, ds_n \tag{2}$$

Shear work is defined mathematically in a similar manner but with tangential forces F_T and over the sliding distance ds_T. Shear work is usually used to predict abrasion and wear on materials, but in this research, it is accounted to be responsible, alongside impact work, for the exfoliation process of the graphite particles.

3. Results

The simulation results found that the power that each vessel requires to maintain its rotational velocities depends primarily on the rotational speed and not so much on the size of the balls. This is an expected result, as the power must be a function of mass and angular momentum, and the mass is fixed along the different ball size cases.

Table 2: Power (W) drawn by the mill to maintain constant angular momenta

Power draw (W)	**Ball size (mm)**		
Angular speed (rpm)	**3**	**5**	**10**
100	3.56×10^{-3}	2.85×10^{-3}	3.03×10^{-3}
300	0.105	9.98×10^{-2}	0.110
500	0.428	0.392	0.442

As shown in Figure 3 a) and b), both shearing and impact collisions are more frequent at high energies as the angular speed increases. Such energies are of greater interest, as are the ones that can break material off and not only deform it or be dissipated into heat. The most desirable speed to work, despite the higher consumption, would then be 500 rpm, as the collisions that this angular speed produces are with high energy and are more frequent. This ultimately leads to less operational time for the apparatus, as it will achieve the desired product comminution much faster.

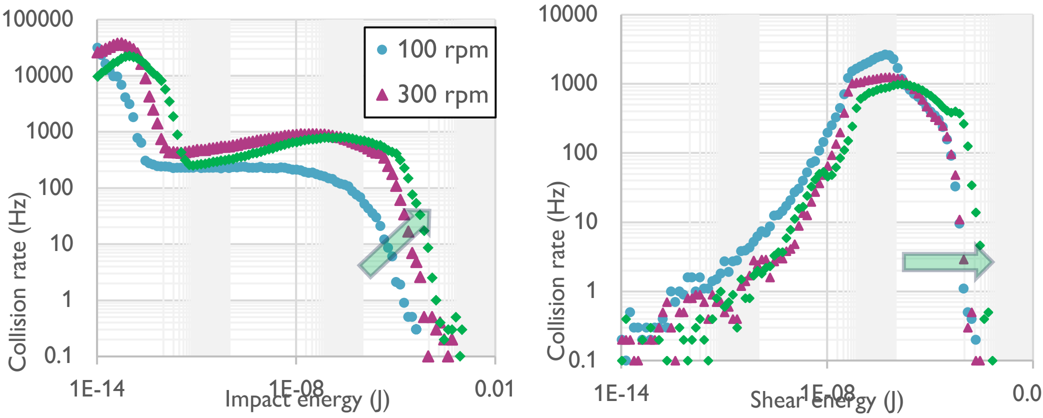

Figure 2: a) Impact energy spectra for 0.5 cm between steel balls at different angular speeds. b) Shear energy spectra for 0.5 cm between steel balls at different angular speeds

All materials have an energetic threshold depending on the particle size that separates "useful" collisions from "not useful" ones that do not produce size reduction. Low energy collisions may be dissipated into heat or just able to break down the smallest dust particles. In this sense, it is more desirable to have high-energy impact collisions as these are destined to reduce the material to the desired size. Not surprisingly, higher angular speed seems to give the most promising results, as 500 rpm provides both high energy impact and shearing collisions more frequently.

Figure 3a depicts how frequent and energetic different types of collisions are. Most of the energy is transferred by collision impacts between balls and against the walls of the vessel. Shearing collisions against the wall seem to be frequent in medium-range energetic levels, which can produce shear stresses on the ground particles, sometimes desired for different types of nanomaterial production (Wang et al., 2023). These shear energy in collisions must be considered carefully, as in many models, they are believed to be responsible for the wear of the grinding materials and the mill vessels. Figure 3b shows the power consumed by each type of collision at each energy level. Although previous figures showed that low-energy collisions are more frequent, the total sum of them is not enough to overcome the energy that goes into highly energetic collisions. Most effective power is dissipated in ball impacts against the wall ranging from $2.9 \cdot 10^{-5}$ to $3.5 \cdot 10^{-5}$ J and in shearing between the balls and the walls at collisions ranging from $7.0 \cdot 10^{-5}$ J to $8.5 \cdot 10^{-5}$ J. While angular speed clearly has a direct effect on the amount of energy that goes into the system, it is not so clear for different ball sizes, as simulations are set up to have similar total masses. The grinding ball size must have an effect not on the amount of energy but on the energy distribution itself and the way the energy is distributed between impact and shearing collisions. Results show that the size of the ball greatly impacts the energy distribution inside the mill.

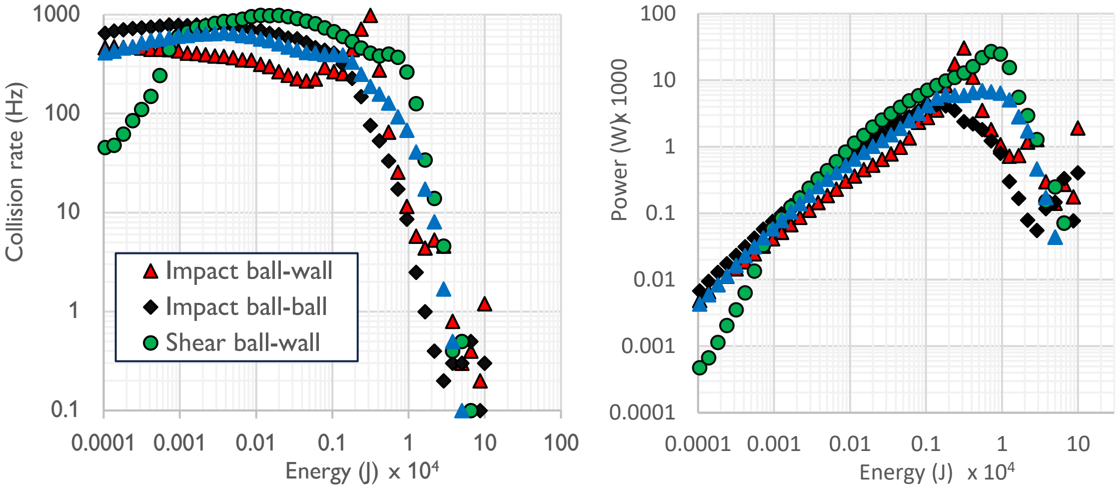

Figure 3: a) Energy distribution, shear/impact for 500 rpm and 0.5 cm balls. b) Power consumption, shear/impact for 500 rpm and 0.5 cm balls

The higher energy impact collisions occur more often only for 0.5 and 1 cm steel balls, while for 0.3 cm balls, more power is dissipated in low energy impacts. To optimize the mill for normal or impact collisions, 0.5 cm balls give the best results among the tests performed. Steel balls with 1 cm in diameter seem to also provide good performance in this matter. When looking at shear energy, it seems that the greater the ball size, the more energy shearing collisions have and the more frequent those are. Steel balls of 1 cm and at 500 rpm produce ~170 shearing collisions per second of more than 10^{-3} J. Figure 4 depicts the internal dynamics of particles inside the mill. At low 100 rpm, the balls suffer the effect of gravity and are placed on the floor of the vessel, while at high revolution speeds, particles stick to the lateral wall of the vessel, producing higher contact forces.

Figure 4: Ball movement inside the mill at different speeds. a) 100 rpm. b) 300 rpm. c) 500rpm

The way in which energy is distributed inside the mill for different ball sizes is a complicated subject. As the angular speed is fixed in all simulations, depending on the mass of the particles, different behaviors may be present, from sticking to the walls to bouncing randomly inside the vessel. For all cases, shear collisions take more total power than impact collisions, as is expected for a planetary ball mill. For 1 cm balls, most energy is dissipated in shearing collisions against the walls, as a lower number of balls makes ball-ball collisions less probable. It is also notable that most of the power is consumed in high-energy ball-wall collisions (10-3 J), while in other sizes, most power goes to (10^{-5} J) ball-wall collisions or (10^{-4} J) ball-ball collisions. The 0.5 cm size seems to draw the most power in highly energetic ball-ball collisions, while the smaller ball sample (0.3 cm) uses similar total power but at lower energy shearing collisions. Some clear trends arise from the results mentioned.

- The larger balls are, the less numerous they become, and they are more likely to collide with the walls than between themselves.
- The smaller the balls are, the less energetic the collisions are, and more power is dissipated in lower-energy collisions.

From all the useful power 65.4 % and 54.0 % go into ball-wall shearing collisions for both 1 cm and 0.3 cm balls. Around 0.5 cm balls, there seems to be a minimum as only 46.7 % goes into ball-wall shear collisions. Despite this, those types of collisions take more power than any other for all the cases studied.

4. Conclusions

Planetary mills have been studied under different conditions, and the results are dependent on the materials and quantities to be milled. If the mill is to be used for impact conditions, the 500 rpm case with 0.5 cm balls seems to give the best results, being more efficient in creating such types of breakage-producing collisions. The 500 rpm case is generally preferred except for cases where the grinding is performed on very brittle materials or where the particle's breakage or deformation must be carefully controlled. For resistant materials, the use of larger balls is desirable, as they create larger collision energies. If shearing collisions are desired, 1 cm balls are the ones that provide the best results for these types of collisions. The power consumption of the mill depends almost solely on the revolution speed of the mill, although the cases with 0.5 cm balls give slightly lower energy requirements than the others. For cases where shearing collisions are undesired, as they can produce wear on the wall and milling balls, the ball that produces less wear is 0.5 cm, with only 46.7 % of the energy being wasted on those collisions. DEM simulations have proved to be a suitable tool for determining the effect of its operation variables, such as the “revolutions per minute” or the size of the balls on the characteristic mill energy profile. This study provides an understanding of the internal dynamics of planetary ball mills, which are key for the development of nanomaterials. Using the optimal processes found in this study will result in an increase in process efficiency and faster production of the ground material. Future work will be focused on the study of the mill conditions with the inclusion of the grinded material. The combination of different-sized balls in a single simulation can also lead to interesting results regarding the efficiency of the mill, as it is the total volume that these balls occupy.

Nomenclature

F – Force (N)
F_n – Normal contact force (N)
F_T – Tangential contact force (N)
m – mass (kg)
s_n – Overlapping distance on normal impact. (m)
s_T – Sliding distance on tangential impact. (m)
t – time (s)
v – velocity (m/s)
W_{imp} – Work made in particle normal impact (J)
μ – Skin friction coefficient (-)

Acknowledgments

The authors would like to thank the financial support of the Mir Puig Private Foundation. Author Jingli Han acknowledges the financial support from the China Scholarship Council (No. 202308410535).

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