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Insights into advanced ball mill modelling through discrete element simulations

Victor A. Rodriguez, Rodrigo M. de Carvalho, Luís Marcelo Tavares*

Department of Metallurgical and Materials Engineering, COPPE, Universidade Federal do Rio de Janeiro – UFRJ, Cx. Postal 68505, CEP 21941-972 Rio de Janeiro, RJ, Brazil

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ABSTRACT

Important advances have been made in understanding ball milling during the last 25 years or so, a great part of it owing to the widespread application of the discrete element method (DEM), which is now an integral part of several advanced ball mill models. These models, however, must rely on assumptions regarding the mill mechanical environment that can help make the problem more manageable. The paper analyzes the validity of some assumptions that have been the basis of several advanced ball mill models by conducting DEM simulations of dry batch mills including both grinding media and particles. The validity of the assumption of perfect mixing of grinding media and particles, as well as of simulating exclusively the grinding media in order to collect the collision energy information for prediction of breakage and, thus, saving computational effort, are analyzed in great detail. It is concluded that the assumption of perfect mixing in the radial direction is generally valid, except for mill frequencies that are unusually high and exceedingly large ratios of mean ball and particle sizes being ground. It is also observed that a fraction of the number of collisions inside the mill do not involve particles, so that an empirical expression that is based on the ratio of surface areas of the ball and particle charge is proposed to estimate such proportion of unsuccessful collisions. Finally, a model from the authorś laboratory, that assumes that each collision in the mill will involve a monolayer bed of particles, is tested, demonstrating reasonable agreement when compared to simulations.

1. Introduction

Mathematical modeling of tumbling ball mills has evolved tremendously over the last 70 years or so. From the empirical size-reduction relationships (Charles, 1957; Bond, 1952; Morrell, 2004) to the traditional population balance model (Austin et al., 1984; Herbst and Fuerstenau, 1980) and the more recent mechanistic models (King and Bourgeois, 1993; Capece et al., 2014; Datta and Rajamani, 2002; Tavares and Carvalho, 2009), several approaches have been proposed, which vary significantly in respect to complexity, fidelity and level of detail in describing the physical phenomena in ball milling.

In recent years, these so-called advanced models have been receiving progressively more attention, given their power to open, at least in part, the "black box" of ball milling through detailed descriptions of the media motion and the corresponding energies involved in the collisions. This has been made possible by the application of the discrete element method (DEM) to ball milling, coupled to some form of population balance model formulation (Tavares, 2017; Weerasekara et al., 2013). Several different approaches have been proposed over the years (Cleary, 2001; Datta and Rajamani, 2002; King and Bourgeois, 1993; Powell et al., 2008; Tavares and Carvalho, 2009; Wang et al., 2012; Capece et al., 2014), with some similarities as well as important differences among them, as recently reviewed by Tavares (2017).

Several of the advanced models of ball mills, as well as other media mills (Beinert et al., 2015), rely on collision energy information from simulations that do not include particles, only grinding media (Datta and Rajamani, 2002; King and Bourgeois, 1993; Tavares and Carvalho, 2009), while others include both grinding media and ore/powder particles (Capece et al., 2014; Powell et al., 2008; Wang et al., 2012). In the case of models that rely on DEM simulations that only contain the grinding media, as well as in every case when grinding of fine particles, called sub-DEM particles (Powell et al., 2008) is to be predicted, a reasonable assumption must be made regarding the mass (or volume) of material captured in each stressing event and how the available collision energy is split among the particles (Datta and Rajamani, 2002; King and Bourgeois, 1993; Tavares and Carvalho, 2009). In nearly all of these approaches it is assumed that every collision in a ball mill will involve particles (sub-DEM particles). Another underlying assumption

* Corresponding author.
E-mail address: tavares@metalmat.ufrj.br (L.M. Tavares).

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considered when only grinding media is included in the simulations is that particle to particle and particle to liner collisions are not sufficient to cause breakage and may be considered negligible in ball milling.

Nearly all workable advanced mill models assume that mills are perfectly mixed in the radial direction. The validity of this assumption has been analyzed using both experiments and simulations. Cleary (1998) inferred, with the aid of DEM simulations, that there are two mechanisms responsible for size segregation in mills: one that operates at low speed and concentrates coarse particles around the outside portion of the charge, and the other that operates at high speeds and that is responsible for accumulation of coarse particles in the center of the charge. He suggested that, at intermediate rotation speeds, the mill charge behavior could be considered perfectly mixed. A later study (Cleary and Morrison, 2011) analyzed the behavior of the charge influenced by the presence of fine particles. The authors concluded that, even with 100% of powder filling, the toe region is not yet packed with powder, with that occurring only at higher percentages. In addition, it was observed that the particles were not uniformly distributed and neither well mixed. However, these authors' research relied on simulations on some particular conditions, that is, a 435 mm diameter mill equipped with six small (8 × 8 mm) lifters, which directly influenced their outcome.

The present work used DEM to conduct virtual experiments to assess the validity of several important assumptions commonly used in advanced ball mill modeling, by including not only grinding media (balls) but also particles (ore/powder) in the simulations. As such, it allowed investigating directly the validity of the assumptions of perfect mixing in a dry batch ball mill as well as the effectiveness of the grinding media when nipping particles.

2. Methodology

2.1. Setup of DEM simulations

The simulations were performed using the discrete element method. This method has been successfully used in different approaches in the field of particulate materials (Barrios and Tavares, 2016; Cleary and Morrison, 2011; Powell et al., 2008; Segura-Salazar et al., 2017), and a detailed description of the method may be found elsewhere (Weerasekara et al., 2013). Simulations were carried out using the EDEM software version 2.7 by DEM Solutions (Edinburgh, UK).

Different mill geometries and operation modes were selected and a summary of the mills and operating conditions simulated is presented in Table 1, whereas a snapshot of the mills simulated is given in Fig. 1. The rectangular shape and the significant height of the lifters used in the 30 cm-diameter mill resulted in onset of cataracting motion with mill frequencies as low as 50% of the critical speed. Nevertheless, simulations were also conducted for shallower lifters in order to assess their effect. In most cases, particles were simulated as monosize. In selected simulations, however, particles were simulated following the size distribution given in Table 2. In addition to the small-scale mills simulated, pilot and industrial-scale semi-autogenous (SAG) mill were also simulated in DEM. A summary of their characteristics is given in Table 3. Although the work was not focused on SAG milling, simulation data from these mills allowed to demonstrate the validity of some of the approaches to larger diameter mills and to other types of media mills.

Both grinding media and particles were simulated as spheres, taking advantage of the convenience and reduced computational demand associated to this simple shape and relying on the limited influence of particle shape in mixing in a ball mill observed by Höhner et al. (2015). A summary of properties of steel grinding media (and mill shell) and particles simulated is given in Table 4.

Simulations were conducted at different values of voids or powder filling, which is defined as percentage of the voids left in the ball charge that are filled with particles, including the voids between them, when the mill is at rest. This is estimated assuming a nominal porosity (voidage) of the ball charge of 40%.

The no-slip Hertz-Mindlin contact model was used in the simulations using the discrete element method. The values of the parameters for steel-particle and particle-particle contacts were collected from a previous study in the authorś laboratory (Ramos et al., 2011), having allowed to match the measured mill power with the simulations. Parameters for steel-steel contacts were gathered from the literature (EDEM, 2016) and are also summarized in Table 5. In the case of DEM simulations with no ore particles, in which the ball charge must describe the movement as if both particles and media are present, the parameters used were 0.6 for the coefficient of restitution, 0.35 for the coefficient of static friction and 0.2 for the coefficient of rolling friction.

In some cases the whole length of the mill (Table 1) was included in the simulations. However, in order to reduce computational effort, only a section of the mill length (slice) was simulated in most cases. Whenever that was the case, periodic boundaries were used, which allowed both grinding media and particles leaving from one boundary appear immediately on the opposite boundary of the simulation. In these cases, the length of the slice was chosen to be equal to at least three times the maximum diameter of the grinding media (Carvalho, 2013; Carvalho and Tavares, 2013; Cleary, 2001; Weerasekara et al., 2016).

Simulations were initially conducted for up to 15 s, guaranteeing that steady-state conditions were reached. After this, information on particles and grinding media positions and collision energies (energy loss values) were recorded during two complete revolutions of each mill studied.

2.2. Post-processing of DEM simulations

2.2.1. Mixing

Two approaches were used in the present work to analyze mixing in the mills. First, an analysis following a microscopic approach using the relative standard deviation (RSD) of the number of particles contained in grids inside the mills was carried out. This method, which has been successfully used in the past (Cleary, 1998; Pantaleev et al., 2017; Seyed-Alian, 2011), basically consisted in dividing the cross section of the mill in a preset number of grids, resulting in a number of bins (Fig. 2). After that, the mean number (x) of ore/powder particles in each bin (whenever any particles were present), as well as the standard deviation (σ) of the simulated data, are calculated. This relative standard deviation is then given by:

$$RSD = \frac{\sum_{i=1}^{n} \frac{\sigma}{x_i}}{n} \tag{1}$$

where n is the number of bins.

The lower the value of RSD, the more uniformly distributed particles are and, thus, the better the mixing of the charge. The spacing of

Table 1
Summary of the small-scale mills and conditions used in the simulations.

Mill	Diameter (cm)	Length (cm)	Filling (%)	Ball size (mm)	% critical speed	Particle size (mm)
A	30	30	20/30	15/25/40	40/50/60/80	1.5–15.9
B	58	24	20/30	15/25/40	40/50/60/80	1.5–15.9