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Original Research Paper

A novel and direct approach for modeling and simulation of impact grinding

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ABSTRACT

A new era of particle breakage simulation has started recently with the advancement in discrete element method (DEM). Prediction of the breakage distribution as a function of specific comminution energy and material characteristics is of great significance for DEM simulations. King (2001) proposed a single parameter breakage model, consisting the parameter t_{10} along with a tuning constant α. In the present study, single particle breakage data obtained from a series of drop-weight tests were fitted into the model to find out the corresponding values of the parameter and tuning constant. The dependencies of these values are studied and mathematically modeled against the specific comminution energies and material characteristics. Methods are suggested to predict the parameter t_{10} with the help of JK model (Napier-Munn et al., 1996). Further, based on the proposed mathematical models, DEM simulations have been performed and validated experimentally. The central idea is to draw a direct approach that can simulate the particle breakage due to impact in a complex grinding environment. Relatively easier ways are discussed to predict t_{10} and α of the single parameter breakage model which makes it a proper candidate for the modeling and simulation purpose. Also, it is reconstituted that α is a material characteristic, reasserting King's model as a single parameter model.

1. Introduction

Single particle and particle bed breakage studies with standard drop-weight and twin pendulum test have been extensively used to determine the comminution energy for breakage [3–8]. A different version of a drop-weight tester known as ultrafast load cell or more recently known as the impact load cell has been used to understand the fracture and deformation characteristics of particles under impact loading [9–11]. Ultra-fast load cells can measure the particle fracture energy, strength and stiffness. King and Bourgeois [12] reported that the frequency distribution of fragments resulting from breakage of single particle or bed of particles obeys the log-normal probability distribution. Statistical average of a number of single particle tests data represents the macroscopic behavior of the system in the form of breakage function [4]. Particle fracture energy in such breakages depends on the material properties and can be estimated from Hertz contact theory [13]. In general, specific fracture energy is preferred over the fracture energy as it includes the parent particle size effect on energy requirements.

Grinding is a kinetic process and the models to represent these kinetics commonly involve parameters such as selection function (S_i) and breakage function ($B_{i,j}$). Selection function is a measure of how fast the material of a given size i breaks, whereas breakage function indicates the distribution pattern of fragments. It is customary to represent the cumulative breakage or breakage function in terms of mathematical models [6,14,15]. Klimpel and Austin [16] proposed a widely accepted breakage distribution model, as given below:

$$B_{i,j} = \varphi_j \left(\frac{x_i}{x_j}\right)^{\gamma} + (1-\varphi_j)\left(\frac{x_i}{x_j}\right)^{\beta} \qquad (1)$$

where $B_{i,j}$ is the cumulative fraction of the material broken from the size fraction j reporting to the sizes below the size fraction i. Model parameters, φ_j, γ and β are material characteristics [17]. The values of φ_j and γ ranges from 2.5 to 5, and 0.5 to 1.5, respectively. β represents the fraction of fines produced in a single fracture event. Despite the simplicity of the model, its parameters lack physical significance [18]. The same is also observed in the present work.

An elegant approach for estimating the breakage distribution was put forward by introducing the t-family of curves [19]. In this approach, the product size distribution (PSD) is represented by a family of curves using marker points (at fraction of parent particle

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size) on the size distribution plot. In a simplified manner, breakage distribution is characterized against a set of t_n values representing the cumulative fraction of fragments smaller than $1/n^{th}$ of the parent particle size. Later, King [1] worked out on t-family of curves and proposed a single parameter empirical model along with a tuning constant, as given below:

$$t_n = 1 - (1 - t_{10})^{\left(\frac{9}{n-1}\right)^{\alpha}} \tag{2}$$

where t_{10} is a model parameter representing the cumulative mass fraction passing $1/10^{th}$ of the parent particle size and α is a material characteristic. The invariable nature of the material over a range of practical or industrial purposes treats α as a constant. Therefore, the model is peculiarly called as a single parameter breakage model.

Tavares [20] proposed t_{10} as a function of specific comminution energy in the form of the equation given below:

$$t_{10} = t_{10(\max)}\left(1 - e^{-\frac{\beta E_{CS}}{E_{50}}}\right) \tag{3}$$

where E_{CS} is the specific comminution energy in kWh/t. β and E_{50} (median impact fracture energy) were considered material characteristics. $t_{10(\max)}$ is also a material characteristic that represents the value corresponding to the plateau of plot between t_{10} and E_{CS} [2]. $t_{10(\max)}$ can be determined by standard drop ball tests at a condition when specific comminution energy is sufficient enough to break 50% of feed mono-sized particles [19]. The measurements of the distribution of particle fracture energies can also be used to estimate $t_{10(\max)}$ [2,15,21]. t_n versus t_{10} relationships can be used to predict the product size distributions at different grind times [14].

JK drop-weight test provides an excellent methodology to test the material resistance towards the impact breakage and abrasion [2]. For a range of impact and abrasion conditions, the appearance or breakage function of the ore is mathematically represented by three parameters such as A, b and t_a. A and b is collectively called impact parameters, and t_a is called abrasion parameter. These parameters are well suited for simulations of AG/SAG (autogenous and semi-autogenous) mills, crushers, HPGR (high pressure grinding rolls) [22]. JK impact parameters, A and b are usually obtained by fitting the JK drop-weight test data into JK model given in Eq. (4). JK model is itself analogous with Eq. (3), where A replaces $t_{10(\max)}$. In JK model, parameter A can attain a maximum value of 60 or 70 and parameter b ranges between 0.1 and 4.0 [22].

$$t_{10} = A(1 - e^{-bE_{CS}}) \tag{4}$$

Substantial efforts have been expended through experimental and numerical work to study the effect of operating conditions on the performance of tumbling mills. However, even after knowing the exact mechanism of breakage, the incomplete knowledge of energy distribution among colliding bodies restricts the advancement in overall understanding of the comminution process [22–24]. There have been several attempts to perform simulations of the impact grinding with the help of experimentally determined parameters [14,25–28]. In such population balance approaches, one or more parameters such as S_i and $B_{i,j}$ determined from experiments are used in simulations to predict PSD at different grind times. However, S_i needs to be determined or back-calculated for any change of operating or design conditions [16,29,30]. At least two parameters of the mathematical models for the prediction of S_i, have said to be dependent on the milling conditions such as mill dimensions, mill speed, ball load and size distribution [17,31,32].

DEM is a computational technique used to simulate the behavior of granular motion [33–38]. The methodology of DEM computations has been described elsewhere [39–41]. There are numerous examples of the wider applicability of DEM for granular simulations. In relevance to present study, Sato et al. [42] have studied the grinding media abrasion rates in a planetary mill against grinding time with the help of energy spectra provided by DEM. Gaudin et al. [43] studied the effect of friction coefficient on media motion in the wet bed mill. DEM was also used to study the complicated particle-bubble hydrophobic interactions in flotation [44].

Cone crusher simulations for compressive breakage of bonded-spherical particles was performed using DEM [45]. In the approach, real particles are three-dimensionally scanned for their geometries, and then computational environment realizes the particles real shape as bonded bi-modal distributions of spheres. Scanning and reproducing a large number of particles discourage the practical implementation of this approach. On the other way, researchers first obtain the ball mill energy spectra with the help of DEM simulations, and then mathematically relate it to the experimental breakage data. Further, non-DEM simulations are performed with the help of developed mathematical models [22,46–48]. A scale-up technique can be used with this method to perform simulations with change in geometrical dimensions. However, the technique may impose limitations, especially in the case of change in a geometrical shape. Otherwise, the energy-spectra needs to be determined on case-to-case basis. Morrison and Cleary [22] have found the energy spectra for impact and abrasion in SAG mill. Then, JK model was used to calculate t_{10} values based on the energy spectra. However, in this approach instead of real values, the values of A and b were assumed at 50 and 1, respectively, and it was suggested to predict the complete size distribution based on t-family of curves. Later, Delaney et al. [49] provided some resolution over these issues by incorporating some complex mathematical models in DEM for different breakage mechanisms.

Therefore, a DEM simulation technique with universal input parameter is the need of time. An approach that is applicable for a wide range of impact grinding mills and there is no need to determine the parameters on case-to-case basis. It is always appreciable to use parameters that are simple, well established. In this study, breakage behavior of five ores is analyzed. Present work validates Eq. (2) proposed by King as a single parameter model, analyzes its applicability and significance of its parameters. The work proposes a mathematical model for α as a function of specific comminution energy (E_{CS}), specimen feed size (χ) and Bond work index (WI). Methods are proposed to predict t_{10}. The values of predicted α and t_{10} are further used in single parameter breakage model to predict the PSD through DEM simulations.

LIGGGHTS is an open source C++ based DEM package derived from popular molecular dynamics code LAMMPS (Large scale atomic/molecular massively parallel simulator) [50]. LIGGGHTS uses Hertz contact model to quantify the forces between colliding particles, the velocity-Verlet integrator scheme to update the particulate dynamics, and Verlet scheme to perform contact detections [50,51]. In the present study, source code of LIGGGHTS is appropriately modified to incorporate the particle breakage features as per the developed mathematical models. The modified source code is used to perform the simulations of impact grinding.

2. Experimental

2.1. Materials

Five different ores such as banded hematite quartz (BHQ), magnetite, quartz, limestone and coal were selected for experiments. Initially, the ore samples were prepared and dry sieved, and then representative mono-sized samples of −18 + 15, −9.5 + 8.0, −6.3 + 5.6 and −4.0 + 3.35 mm were prepared. The Bond work index of BHQ, magnetite, quartz, limestone and coal are determined by standard Bond's mill test [52].