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Investigation of Breakage Rate Variation of Particle Beds Using DEM Simulation

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Abstract

It has been shown that breakage rate follows the first order kinetic only for a short time at the beginning of grinding process. Thus, most of the available discrete element models (DEM) to model the grinding process are adversely affected as they rely on accurate determination of breakage rate value for their calculations. To present a solution, current study aimed to develop a DEM model which directly applies the particle breakage into the simulation. At each impact event if particle is considered to be broken, the determined fragments are replaced with original particle, as very similar to real grinding environment. To validate the developed model, a grinding ball impacting an unconfined particle bed was simulated at different impaction energy. Energy distribution, breakage rate and particle size evolution were examined. It was shown that fines accumulation led to deceleration in top size breakage rate. The deviation of breakage rate from the first order kinetic was highly effected by impaction energy. A model representing the time dependent breakage model was tested to take into account the impaction energy role. The results proved that there is a need for DEM models which can simulate the grinding process similar to its real environment, with adequate accuracy and independent from the variation of breakage rate.

Keywords: Particle bed, Breakage models, Breakage kinetics, Discrete element method

1. INTRODUCTION

Discrete Element Method (DEM) is a computational method that can provide dynamic information, such as the trajectories of and transient forces acting on each individual particle, which is extremely difficult to obtain by physical experimentation. DEM has been used to investigate several different aspects of mill performance. Particle breakage, surprisingly, is of the least investigated areas of mill performance using DEM whilst it is, indeed, the most basic and fundamental part of the grinding process. Grinding process is a complex process which always includes different modes of particle breakage and shape change. Necessity of taking account theses modes in DEM modelling of comminution is one of the main reason which makes the modelling of grinding to be challenging and less attention paid. The DEM combined with the single-particle breakage approach allows the detailed physics of the process to be incorporated in the modelling of the breakage process.

Despite all devoted effort in simulation and understanding of the particle breakage in milling process (Datta and Rajamani, (2002); Capece et al., (2014); Kalman et al., (2009)), there is still a long way to go. Simulation results including produced PSD do not fairly correspond to experiments. As our knowledge of breakage and computational capacity improve, it is possible to include increasingly realistic descriptions of the breakage process directly in the DEM model. In this study, a novel method to simulate the particle motion and its breakage simultaneously in packed beds has been proposed. It directly implements the particle breakage

inside the DEM computation algorithm and if any breakage happens the original particle is replaced with progeny. In this way, the calculation will be followed based on a new updated particles list which is very similar to real grinding environment. So, it would be able to determine the particle breakage and its distribution.

2. MODEL DEVELOPMENT

2.1. DEM model

An in-house developed DEM model is used in current study. In DEM simulations, the motions of a particle of radius R_i and mass m_i is described by (Zhu et al., (2007))

$$m_i \frac{dv_i}{dt} = \sum_j \left(F_{ij}^n + F_{ij}^s\right) + m_i g \tag{1}$$

$$I_i \frac{d\omega_i}{dt} = \sum_j (R_i \times F_{ij}^s - \mu_r R_i \left|F_{ij}^n\right| \widehat{\omega}_i) \tag{2}$$

where v_i, ω_i and I_i are, respectively, the translational and angular velocities, and the moment of inertia of the particle. R_i is a vector running from the centre of the particle to the contact point with its magnitude equal to particle radius, and μ_r is the coefficient of rolling friction. F_{ij}^n and F_{ij}^s represent, respectively, the normal contact and tangential contact forces imposed on particle *i* by particle *j*.

2.2. Modeling particle breakage

2.2.1. Breakage probability determination

The energy distribution in the mills is investigated in term of the collision energy. At each impact event, the impact energy induced on particle was calculated. The mass specific collision energy is calculated by $W_m = \frac{1}{2} V_{nij}^2$, where $V_{nij}=V_{ni}-V_{nj}$ is the relative normal velocity of particle and grinding ball at the collision event. The model implemented here, makes decision about the particle breakage at each impact event, individually. Therefore, considering k=1 (k is the number of impact) the following form of the Vogel and Peukert, (2003) has been applied here.

$$S = \begin{cases} 0 & W_m \le W_{min} \\ 1 - exp[-f_{Mat}.d.(W_m - W_{min})] & W_m > W_{min} \end{cases} \tag{3}$$

where S is breakage probability, W_m and W_{min} are the mass specific energy and minimum mass specific energy required to break a particle and d is the feeding particle diameter and f_{Mat} is a fitting parameter. For those energies (W_m) less than W_{min}, particle fracture or deformation will not happen. W_{min} is a size dependent material property. Vogel and Peukert, (2003) determined that the product $d.W_{min}$ is a constant material property ($d.W_{min}$=*constant*).

2.2.2. Determination of fragment size distribution and position

If the particle cannot resist against collision then it is split into fragments, so breakage function is needed to determine the size distribution of the breakage. We applied here the

Vogel and Peukert, (2002) breakage function without considering the term for very fine progeny. The cumulative volumetric breakage function *B* can be expressed by:

$$B_i = \left({}^{d_i}/_{d_b} \right)^{\alpha} \tag{4}$$

$$\mathrm{a} = \mathrm{A}\,.\ln(\mathrm{d}.\mathrm{W_m}) + \mathrm{B} \tag{5}$$

where B_i is the cumulated mass fraction for fragments of size below size class of the broken particle. To needs to be mentioned that here we are dealing with single particle breakage. Therefore, for each sub size class, the fragments will be received only from the broken particle size. d_b is the size of the particle subjected to the breakage part and 'α' is an empirical parameter that takes into account the effect of the impact energy (W_m) and particle size. d_i is a virtual sub-sieve size which denotes on considered size classes for fragments. It has been pointed to be $0.5d_{init}$, $0.25d_{init}$, $0.16d_{init}$ and $0.1d_{init}$ where d_i is the feed's initial size. It was found out that the relation between the α and d and W_m can be stated as Eq. 5, where A and B are the model parameters. Using breakage function, the percentage of material remained on each sub-sieve size is determined. Then amount of retained mass on each sieve is converted to particle number

2.3. Simulation conditions

At the beginning of the simulation, a bed of particle consisting of 50 limestone particles with 25.4 mm diameter is formed at top of the square based with 101.6 mm × 101.6 mm and periodic boundary conditions. Then, the packing process proceeded until all particles reached their stable positions with essentially zero velocities as a result of the damping effect for energy dissipation. Once bed formation was completed a steel ball with 76.2 mm diameter was released from a specified height to fall down vertically and hit the particle bed. 4 simulations have been carried out. The difference between them was in the amount of grinding ball vertical velocity at the time of reaching on the bed surface. To do so, the grinding ball height from the bed surface and its initial velocity has adjusted in different ways. The vertical velocity of grinding ball determined to be 10.8, 7.7, 4.7 and 3.5 for simulation#1, 2, 3 and 4, respectively. Grinding ball was intended to hit the particle bed only once at every 0.5 s. Thus, collision data were not collected when the steel ball rebounded from the particle bed. Fig. 1 shows the general view of the simulations and Table 1 shows the applied parameters in DEM simulation and their values.

Experiment data conducted by Tuzcu, (2010) was taken to determine the applied functions' parameters. Fitting revealed that f_{Mat} and $d.W_{min}$ values were 9.24 and 0.0214, respectively. Having the $d.W_{min}$, one can determine the amount of the W_{min} for any other particle sizes. It was found out that a logarithmic model well fit on the results. Thus, the relation between a, d and W_m can be stated as:

$$a = -0.353\ln(d \times W_m) + 1.93 \tag{6}$$

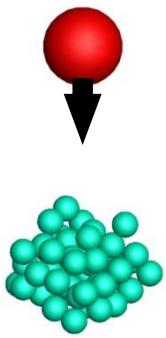

Figure 1. A view of the simulation set up

Table 1 Parameters and their values in the DEM simulation.

Parameters	Steel balls	Limestone Powders
Density, $\boldsymbol{\rho}$ ($^{\boldsymbol{kg}}/_{\boldsymbol{m^3}}$)	7.8×10^{3}	2.58×10^{3}
Young's Model, $\boldsymbol{Y}$ ($^{\boldsymbol{N}}/_{\boldsymbol{m^2}}$)	1×10^{7}	1×10^{7}
Poisson's ratio, $\boldsymbol{\sigma}$	0.4	0.4
Sliding friction, $\boldsymbol{\mu}$	0.45	0.75
Rolling friction, $\boldsymbol{\mu_r}$	0.02	0.02
Normal damping, $\boldsymbol{\gamma_n}(\boldsymbol{S^{-1}})$	1.8×10^{-5}	3×10^{-5}

3. RESULTS AND DISCUSSION

3.1. Collision energy distribution

Collision distribution can be used as an indicator to enhance the understanding of grinding environment and interactions among particles. Fig. 2 shows the collision energy distribution based on the different impact for simulation#2. It can be found out the maximum collision energy for this simulation is about 1.3 J. It is also can be seen that the number of high energy collision decreases by progressing the time which due to particle breakage and replacing more coarse particles by fine particles. It needs to be mentioned that for the simulation, only collision energy of impacts happened by particle-grinding ball were collected from the beginning of grinding ball descending to the time that ball starts to be rebounded.

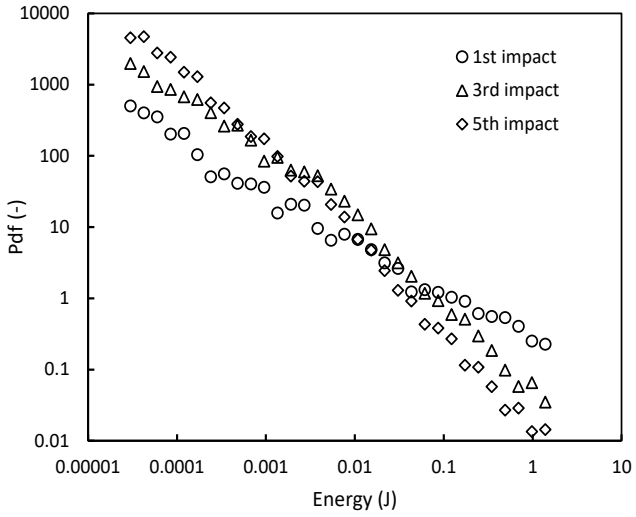

Figure 2. Probability distribution functions of collision energies at different impacts.

3.2. Breakage rate

One of the main factors linked to every grinding process which needs to be determined is the rate at which particles are broken. Traditionally it has been stated that the breakage rate from a given sieve size can be described by (Austin, (1971)),

$$ln\left[\frac{m_i(t)}{m_i(0)}\right] = -S_i t \tag{7}$$

where $m_i(0)$ and $m_i(t)$ are the initial weight and weight retained after *t* grind time, and S_i is the rate of breakage parameter for size class *i*. Some believe that fines accumulation can accelerate or decelerate the breakage rate by changing the inter-particle interaction mode. Hence, a time-dependant model introduced (Bilgili and Scarlett, (2005)) to represent the real breakage rate variation.

$$m_1(t) = m_{1init} e^{\left[-S_{1init} t\left(1+\frac{\lambda t}{2}\right)\right]} \tag{8}$$

As the investigating of breakage rate of the top size class has a high significance, the Eq. 8 has been written for this size class, where S_{1init} is the specific breakage rate when t=0, λ is the parameter which determine the acceleration or deceleration (i.e. $\lambda > 0$ shows the acceleration and $\lambda < 0$ shows the deceleration in breakage rate). The absolute value of the λ also shows the magnitude of deviation from first order kinetic (i.e. higher absolute value=higher deviation). $\lambda = 0$ reproduces the time independent breakage rate relation, introduced in Eq. 10.

The breakage rate variation of carried out simulations at different impact energies has been shown in Fig. 3. It can be seen from the figure that all graphs consist of the two main parts, i.e. linear and non-linear parts. It means that at the early time of the grinding the breakage rate of coarse particles is time-invariant (linear part) but after a while it changes to be time-variant (non-linear part). Non-linear part of the graphs shows that the breakage rate of coarser sizes decreases with time. Eq. 8 was fitted on data. Results of fitting can be used to better explain of the graphs' variation. It was found that S_{1init} is 1.1, 0.47, 0.26 and 0.17 min^{-1} for simulations #1-4, respectively. It means reducing the imposed energy on the particle bed decreased the number of breakage led impacts.

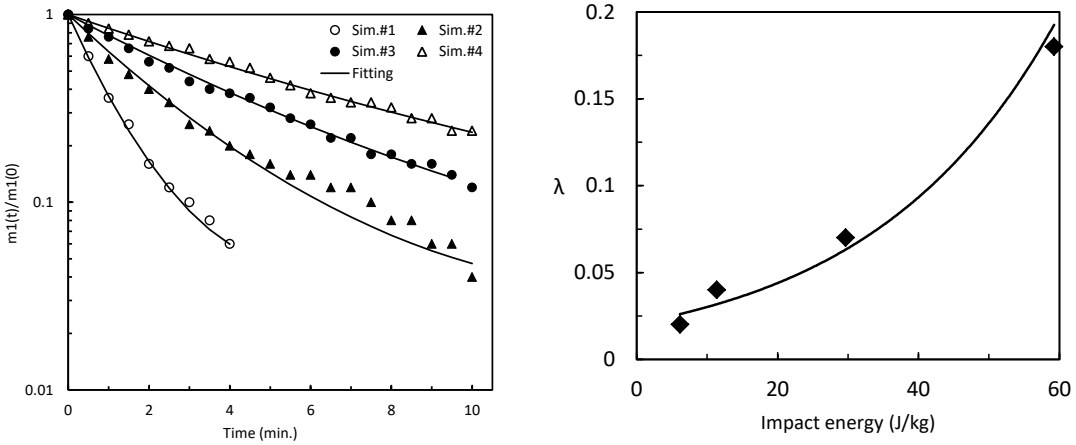

Figure 3. left) Rate of disappearance of the top size class (simbols: simulation results, line: fitting Eq. 8), raight) Variation of λ against the imposed energy (line for guide)

The obtained values from the fitting for λ were graphed against the imposed impact energy on particle bed by grinding ball in Fig. 3. The imposed energy can be calculated by $E = \frac{1}{2}V_{vb}^2$ where V_{vb}^2 is the vertical velocity of grinding time when it touches the particle bed. It can be said from the data that, in all cases coarse particle breakage rate experienced a deceleration by time progressing as the λ<0. Moving from high impact energy grinding environment (i.e. sim.#1) to low impact energy (i.e. sim.#1), the deviation from first order kinetic decreased as λ absolute value decreased. By an exponential fitting the relation between λ and E_{im} for simulated cases found to be $\lambda = 0.021\exp(0.038E_{im})$.

4. CONCLUSION

This study has developed a DEM simulation model which directly applies the particle breakage into the simulation. At each impact event if particle is considered to be broken, the determined fragments are replaced with original particle, as similar to real grinding environment. To validate the model, 4 simulations were carried out to simulate the breakage of a particle bed under impaction of a falling grinding ball at different impact energies. Investigating the energy distributions, breakage rates, and PSDs proved breakage rate follows first order kinetic only at the early time of the grinding. It then shows deviation from first order kinetic. It was shown that there is a direct relation between the magnitude of the imposed energy on particle bed and deviation of breakage rate from first order kinetic. Existing model for representing the time-dependent breakage rate was examined to include the impact energy. Results proved that there is a great need for a DEM model which could simulate the grinding process similar to its real environment, with adequate accuracy and independent from variation of breakage rate.

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