Investigation of Composition Dependent Breakage in High Pressure Grinding Rolls (HPGR) using a novel Breakage Model in Discrete Element Method (DEM) Simulations

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Abstract. The discrete element method (DEM) has been extensively used to model and investigate comminution, but few models consider the materials composition and microstructure during breakage events. Additionally, the interactions between different material phases during comminution are not yet well understood. Since experimental investigations of these relationships are complex and time-consuming, a texture inheritance model for particle breakage in the DEM has been developed. The model uses spherical particles to reduce computation costs which allows simulations with larger quantities of particles, while also conserving particle texture in breakage events. Using the developed texture and texture inheritance model, the breakage behaviour of an artificial magnetite-iron ore is investigated in high pressure grinding rolls (HPGR). By implementing and varying a composition dependence of a peak force breakage criterion, the effects of particle composition on comminution and liberation are investigated. Material with lower critical breakage strength results in more fines and liberation in the product due to more breakage events. Effects of the composition dependent breakage criterion were not observed, likely due to model limitations and a mismatch between comminution and mineral microstructure.

1. Introduction

Discrete element method (DEM) simulations are increasingly used to investigate and optimize processes in the field of granular materials, specifically with the increasing ability to model systems at industrial scale due to improved parallelization strategies, e.g. GPU based calculations, or computationally efficient scaling models, e.g. coarse graining approaches. This brings opportunities to investigate more complex topics that are experimentally time consuming and costly or entirely unfeasible.

In the field of comminution or particle breakage on the discrete level, the mode of breakage is a subject of ongoing discussion. Cracks forming predominantly intergranular could potentially result in better liberation behavior and reduced energy consumption of comminution processes. Additionally, it could increase the size of liberated material which in turn increases the efficiency of subsequent separation processes or enables entirely different ones. While experimental investigations give insights into fundamental breakage mechanisms, transfer to processes on industrial scale is challenging: the investigations are time consuming and changing materials or process geometries demand numerous examinations.

Modelling these mechanisms and incorporation them into a DEM simulation is a way to bridge the gap to industrial processes. Experimental investigations can be used to validate the fundamental breakage behavior of models to ensure realistic representation and the fast adaptability to changing geometric constraints and materials of simulations can be used to facilitate product and process design.

However, consideration of material microstructure in DEM simulations is sparse so far and only considered in set-ups using non-spherical particles. DEM simulations using non-spherical particles have costly contact detection schemes and limited compatibility with coarse graining approaches both of which complicate the application to larger industrial system.

Breakage of spherical particles is usually modeled using the particle replacement method (PRM), which replaces a breaking particle by an array of fragments within the volume of the parent. Volume conservation is ensured by overlapping or shrunk fragments that subsequently push nearby fragments or particles aside or by growth procedures. These replacement schemes inherently pose a challenge for texture considerations: the texture information in void spaces between shrunk fragments is lost or duplicated in schemes with overlapping fragments. To circumvent this, the texture inheritance model was proposed [1]. In the model, a particle's texture is transformed to a cubical shape during breakage events. The cubical texture can be fragmented into cubical fragments without generating overlaps or void spaces. Subsequently, the textures are transformed back to spherical shapes which can be used in the replacement scheme. Previous investigations have shown good agreement of the model with random sampling in varying size classes, indicating the conservative properties of the model with regard to texture.

In this work, the application of the aforementioned model is tested in an industrial scale comminution process. A sensitivity study for the link between the composition of individual particles and their critical breakage strength is performed to investigate a simple connection of microstructure and breakage behavior. The results of the study are a first step in representing the complex interactions of microstructure and breakage

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behavior in breakage models for spherical particles in DEM simulations.

2. Methodology

2.1. Discrete element method (DEM)

The DEM is a Lagrangian numerical approach in which states of individual particles, such as position, velocity, and forces acting on them, are progressively modelled using time steps. To calculate the motion of particles and update their position accordingly Newton's and Euler's equations are solved. To model particle contacts the linear-spring-dashpot model is used [2].

2.2. Texture model

To enable a dependence on the composition of individual particles, the information of the particle's composition needs to be available. The composition of particles in this context is the volumetric parts of individual phases i compared to the total volume of the particle $C_i = \frac{V_i}{V_{total}}$.

However, to accurately model the inheritance of it to fragments in breakage events the microstructure is relevant. In this work, the particles' microstructure is represented as a voxel grid. A low-resolution example of such a grid is shown in Figure 1 (left). Each voxel in the grid is assigned a phase information. The composition can then be calculated as the number of voxels of a phase relative to the total number of voxels in the grid $C_i = \frac{V_i}{V_{total}} = \frac{N_i}{N_{total}}$. The number of voxels, i.e. the resolution, defines the accuracy with which the model is able to represent the texture volume. The texture volume is a digital representation of a real material and can be voxel based, e.g. similar to the slag texture in [1], or more abstract as positions of grains, e.g. the parameterizations by Wiegel [3] or Hilden & Powell [4]. The sampling procedure places the voxel grid of individual particles at random positions within the texture volume. The voxels within the grid then get assigned the phase in the texture volume they are closest to. An exemplary binary texture of a particle is shown in Figure 1 (right).

In this work, an artificial magnetite-iron ore texture following Hilden & Powell [4] is used as texture volume.

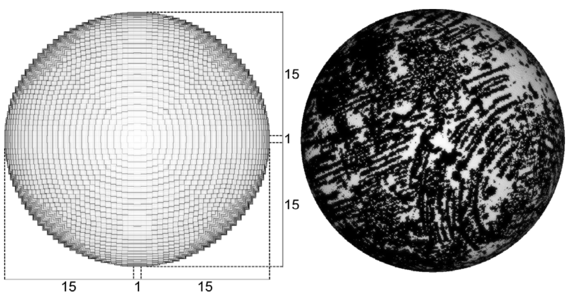

Figure 1. Depiction of a low-resolution voxel-grid (left) and an exemplary high-resolution binary particle texture (right).

2.3. Breakage and texture inheritance model

The breakage model used in this work is an implementation of the previously proposed texture inheritance model [1]. In the model, particles are replaced by an array of spherical fragments within the volume of the breaking parent particle similar to other particle replacement method schemes. Volume conservation is ensured by uniformly shrinking and subsequently growing each fragment. The growth of the fragments is an iterative procedure during which the size of the fragments is increased in small increments if resulting overlaps with surrounding particles, fragments or walls do not exceed a threshold. The growth procedure continues until the fragment reaches the volume required for volume conservation. The threshold needs to be carefully calibrated to ensure resulting forces are large enough for fragments to generate the space necessary for their growth while remaining as small as possible to limit artificial energy input and the influence of the growth procedure on comminution behavior.

Usually, the void spaces between the spherical fragments in the replacement scheme impede the inheritance of texture since the texture information within the void spaces is lost. The previously proposed texture inheritance model [1] solves this issue by intermittently mapping the texture information of the parent particle to a cubical texture using transformations by Roşca et al. [5]. The cubical texture of the parent particle can be fragmented into cubical textures for the fragments without generating void spaces or overlaps. These textures are transformed back to spherical shapes which represent the inherited textures of the fragments. For more details see Hirschberger et al. [1].

2.4. Composition dependent breakage criterion

Cleary & Sinnott [6] use a list of discrete critical breakage forces for each individual size class as breakage criterion (see orange dots in Figure 3). An exponential function can be fit through these values to create a more versatile, size dependent breakage criterion $F_{CS}(x_p)$. The resulting breakage criterion, i.e. the critical breakage force as a function of particle size, is shown in Eq. (1) and Figure 3.

$$F_{CS}(x_p) = a \cdot x_p^b + c, \tag{1}$$

where a, b and c are fit parameters. Equation (1) is the basis of the size and composition dependent breakage criterion used in this work (see Eq. (2)). To include the influence of different phases, a term is created for each phase. Each of these terms describes the breakage strength of the phase using weightings of the size dependent breakage criterion $F_{CS}(x_p)$. The terms are weighted by the volumetric part of the phase C_i in the particles and the strength of the phase relative to the strength of a reference phase $f_{rel,i} = \frac{\sigma_i}{\sigma_{ref}}$:

$$F_{crit}(x_p, C_i) = \sum_i (F_{CS}(x_p) \cdot C_i \cdot f_{rel,i}). \tag{2}$$

In the binary case, i.e. a target material embedded in a matrix, Eq. (2) can be simplified to:

$$F_{crit}(x_p, C_{target}) = F_{CS}(x_p) \cdot (1 - C_{target}) + F_{CS}(x_p) \cdot C_{target} \cdot f_{rel,target}. \tag{3}$$

2.5. Simulation set-up

The simulation used to investigate the performance of the novel breakage model and the influence of composition dependence on breakage behaviour, is a recreation of the simulation by Cleary & Sinnott [6]. The high pressure grinding rolls (HPGR) are modelled using two opposing rolls with a chute above. The chute is filled with particles to feed the system with material. During the entire process the gap between the rolls remains constant and at the pinch-point the gap between them is 60 mm. The rolls rotate with a speed of 19.0 rpm and push the particles into the pinch-point to increase pressure and initiate breakage. A slice in the center of the mill sufficiently large to model particle particle and particle wall interactions is modelled. The slice has a thickness of 189 mm and uses periodic boundary conditions in y-direction. A depiction of the set-up of the simulation is shown in Figure 2 for the initial state.

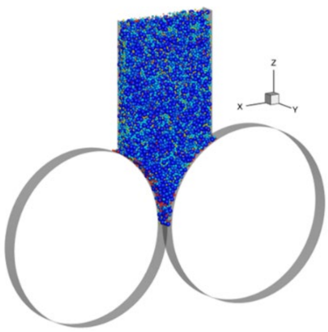

Figure 2. Simulation set-up of the HPGR with the chute filled with feed particles in the initial state.

Material properties of the bulk material used as feed are taken from [6]. For the microstructure, the following relative grain strengths were investigated in the composition dependent breakage criterion (Eq. (3)): $f_{rel,target} \in \{0.5, 1.0, 2.0, 4.0, 6.0, 13.21\}$. The value 1.0 represents the reference case using the strength used by Cleary & Sinnott [6] and the value 13.21 approximates the strength of magnetite grains (extrapolated from the values reported in [7]). Figure 3 shows the critical breakage forces of the particles for the various grain strengths as a function of particle size for an average particle composition $C_{target} = 0.233$.

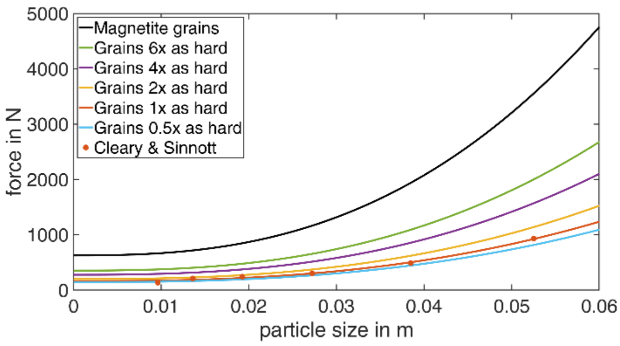

Figure 3. Critical breakage force as a function of particle size for different grain strengths at an average composition of $C_{target} = 0.233$.

To attempt to isolate the effect of the composition dependence in the critical breakage force on the breakage behavior, two additional cases were investigated. In these cases, for the strength of the grains similar values to the matrix material were selected, as is the case in the reference case using Cleary & Sinnott's [6] material properties. However, the strength of matrix and grain material is set to match the average material strength of the composition dependent cases using relative strength values for the grains of 4 and 13.21, respectively.

3. Results

Figure 4 shows the product size distributions of the different grain strengths. For grains with lower critical breakage strengths more fines are produced because more breakage events occur. A corresponding effect for the coarse material is less clear. Since few particles are in the larger particle size classes, larger fluctuations between the strengths are present.

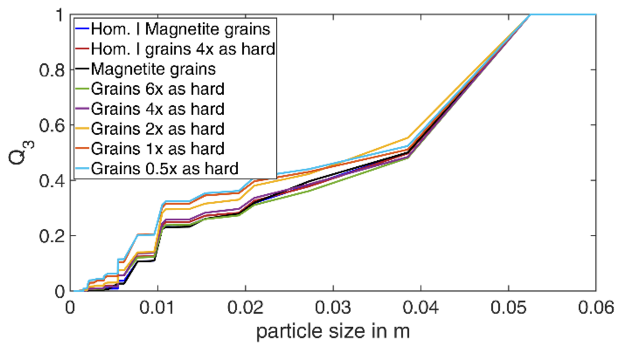

Figure 4. Product size distribution for the various grain strengths.

The size distributions of materials with homogeneous particle microstructures and their composition dependent counterparts show similar size distributions (blue and black, and purple and red curves, respectively). This indicates that the product size distribution is largely independent of the materials composition in the current set-up.

If the forces within the process are significantly larger than the critical breakage forces of either phase, the impact of composition dependence on the comminution behavior would be significantly reduced. For this reason, simulations with stronger grains (four times the strength of the matrix material) and the strongest grains (13.21 times the strength of the matrix material) were used in these investigations. In the simulations with stronger grains, breakage is reduced, which can be observed in the reduced fines in Figure 4. This indicates that the stress in the process is not significantly larger than the material strength. However, relevant difference between the homogenous and composition dependent case were not observed.

The progression over time of the liberation degree of the matrix material in the product is shown in Figure 5. The values approach a constant value after an initial rise, i.e. a stationary process is reached after enough material has exited the domain. Liberation degrees remain low for each grain strength, indicating that the size reduction is not sufficient to liberate the material. Material for which the grains have lower breakage strengths systematically results in higher liberation degrees of the matrix material. Since liberated particles are primarily found in smaller particle size classes, cases with more fines result in higher liberation degrees. As observed for the product size distribution shown in Figure 4, the liberation degrees of materials with homogeneous particle microstructures and their composition dependent counterparts are similar (blue and black, and purple and red curves, respectively). In this set-up the liberation degree of the matrix material appears to be independent of the particle composition.

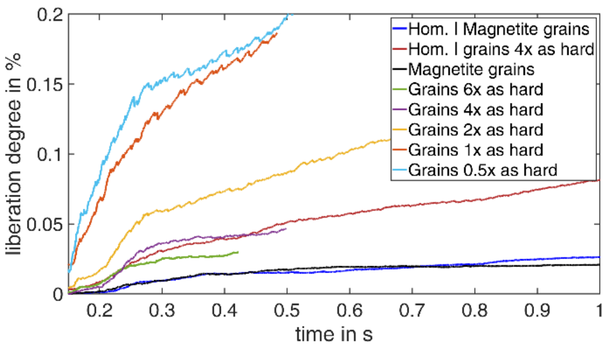

Figure 5. Liberation degree of matrix material in product particles over time for the various grain strengths.

Figure 6 shows the recovery of target material (grains) over the recovery of the matrix material. The angle bisector in the graph represents ideal mixing, i.e. the particles' microstructure does not undergo fundamental changes due to comminution. Weaker materials show marginally more deviations from the angle bisector, but overall the effect of the comminution on the microstructure appears negligible. The comminution in the HPGR set-up is therefore insufficient to liberate the grains for the modelled microstructure.

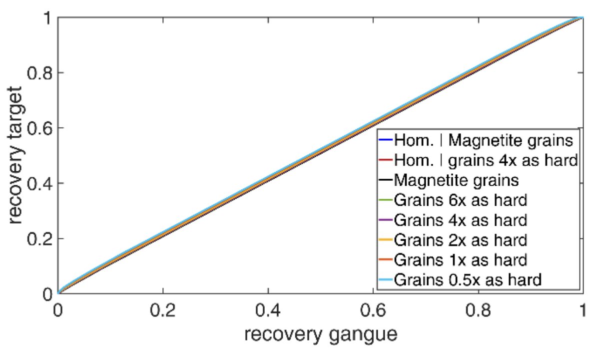

Figure 6. Recovery of target material over the recovery of gangue material for the various grain strengths.

4. Conclusion

The model was shown to be applicable to an industrial scale comminution process. Microstructure information of product material was investigated using size distributions and liberation degrees.

In the comparison of cases using homogeneous particle microstructures and those using a magnetite iron ore texture with a composition dependent breakage criterion only minor differences were observed. An effect of particle microstructure and composition dependence on product size distribution and liberation degree is expected due to the different breakage behavior of liberated particles of the respective phases.

As mentioned previously, composition dependence affects breakage behaviour when the composition of particles changes. Figure 6 indicates that the majority of the mass in the process does not undergo such changes. A more prominent effect of the composition dependence could potentially be observed in processes resulting in more liberation using e.g. a smaller gap size or by using a microstructure with larger grains.

Another aspect is a limitation to two generations of fragments in the employed breakage model. Changes in the breakage behaviour due to the composition dependence, such as weaker material breaking more often, can only be represented in the simulation, if the particles are able to break. However, fragments of the second generation cannot break in the current implementation of the model and any effects of changes in the composition of these fragments on the breakage behaviour cannot be observed in the simulation.

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