

# A Breakage Model for DEM based on a Probabilistic Particle Replacement with Voronoi Fragments

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## Keywords

- Particle breakage
- Comminution
- Polyhedral particles
- Discrete Element Method
- Progeny distribution

## Highlights

- A replacement strategy with pre-defined breakage patterns is presented.
- Progeny distribution can be predicted with high accuracy.
- Mass and volume remain constant and multiple breakage can be simulated.
- Polyhedral particles of any shape can be used.
- The model was validated with various trials with different batches of sinter.

## Abstract

Due to mechanical stress, bulk material is crushed and fines are produced. This can either be desired in comminution processes or undesired in conveying and storage processes. In this work a novel breakage model for the Discrete Element Method is presented to allow a prediction of the resulting particle size distribution after damaging events. The breakage model is based on a probabilistic particle replacement strategy. Depending on the load, the initial particle is replaced by a breakage pattern tessellated with the Voronoi algorithm. Replacement probabilities and breakage patterns follow results from breakage tests. In contrast to other replacement models, mass and volume remain constant. Initial particles are polyhedral and can be of any shape. Crushing processes with multiple breakage can be simulated. The computational scheme is described in detail. The model was verified and validated with trials of shatter tests and two conveying processes with blast furnace sinter from two different industrial partners.

## 1. Introduction

The Discrete Element Method (DEM), originally proposed by Cundall and Strack [1], is a powerful tool for investigating phenomena occurring at the scale of particle diameter and simulating bulk behavior. Thus, DEM has become widely established as an efficient method addressing a variety of engineering problems with granular and discontinuous materials like granular flows, powder mechanics or comminution [2–4].

In many processes mechanical degradation or breakage occurs, so the phenomena cannot be described by DEM alone. When particle breakage does not affect flow or bulk material behavior, DEM and breakage can be decoupled, so that breakage can be investigated in a post-processing procedure. An approach where the compressive force is evaluated after simulation is described in [5, 6]. Another example of decoupling DEM and breakage is a population balance model used for different types of mills in [7–10].

In some cases, particle breakage affects flow or bulk behavior of the material, so that an embedded description of breakage in DEM is necessary. This is the case in various systems, especially in comminution processes [11–14] and transport or storage processes of blast furnace sinter [15–17], for example. Material degradation and fines generation could lead to air pollution, risk of dust explosions, high costs and emissions. This is particularly the case for blast furnace sinter handling because fines have to be re-sintered again, which is a highly energy demanding process. Minimizing material degradation during conveying processes would lead to a major cost reduction and massive savings in energy and CO<sub>2</sub> emissions [17–19].

Different approaches have been developed to describe breakage embedded in DEM. These can be grouped into those in which the progeny fragments are resolved throughout the DEM simulation and those in which fragments only appear when a critical condition is met [20]. The most established model for the former group is the Bonded Particle Model (BPM) [21], which is well suitable to mimic the behavior of agglomerates containing of cemented granular materials [22–28] and has also been used for mills [29, 30] and crushers [31] or even dynamic belt simulations [32]. Further examples for the former group are the Bonded Cell Method [33] and the Discrete Grain Breakage Model [34].

The second group is represented by particle or fragment replacement methods [35]. In the Particle Replacement Model (PRM), originally proposed in [36, 37], the particles are “instantaneously” (within the duration of one time step) replaced by several smaller progeny particles when the criterion for failure is met. The progeny particles can be spheres or clumped spheres [11, 12, 35, 37–40], superquadrics [41] or polyhedral cells [42–45]. The failure criterion could be the excess of a critical force, for example. A major benefit of the replacement method is that the progeny sizes can be defined, so any fragment size distribution can be achieved. Another advantage is that no additional calibration is needed like for other breakage models, such as the BPM.

The particle replacement approach was used to describe particle breakage under confined conditions [38, 46, 47], geotechnical applications [48] and comminution equipment including different types of crushers [12, 13, 41, 49]. The vast majority of PRM uses spheres as progeny particles for computational efficiency. The major disadvantage hereby is, however, the volume loss when a large sphere is replaced by several smaller spheres. To ensure mass constancy, the fragment density was adjusted in [50], which is negligible in mills and crushers, but less suitable for conveying processes because flow behavior and loads on conveying equipment would be distorted. In the work of Tavares et al. [20] volume and mass constancy is ensured by overlapping the following smaller

spheres and defining damping factors for the following time steps to avoid explosions. Further limitations of spherical particles are the description of particle shape and applications when multiple breakage or further breakage of fragments occurs, which is not the case for polyhedral particles [51]. On the other hand, the replacement by spheres is advantageous in terms of computational efficiency. With spherical particles the smallest effort in contact detection and force calculation is necessary and a straight forward conversion to size distribution is possible [51].

Based on the Tavares Breakage Model [52], a model was implemented in DEM in [53, 54] where the Voronoi subdivision algorithm [55–58] is used for mass and volume conservation, which was validated in [59] for single particle drop weight tests. In [45] breakage tests were simulated using polyhedral particles and Voronoi tessellation. Potapov and Campbell introduced a model involving polyhedral particles in [44, 60] called the Fast Breakage Model (FBM). It was used to describe breakage in particle beds in [61, 62] and to simulate comminution equipment in [43, 63]. A comparison of the BPM, PRM and FBM is provided in [64]. In the Discrete Breakage Model (DBM), which is based on [60, 65], the particles are discretized into a number of elements of simple geometrical shapes. The DBM was validated in [66].

In this work a breakage model is presented, which uses polyhedral particles and probabilistically replaces these with Voronoi tessellated breakage patterns if a critical condition is met. The model was first presented in [67–69] and is described in detail in [70] which is a PhD thesis in the evaluation process at the time of writing. The model allows to simulate particle breakage embedded in DEM. Various processes like conveying or comminution processes can be simulated efficiently in order to predict the resulting particle size distribution (PSD) with high accuracy.

## **2. Single particle impact tests**

For detailed investigations of particle breakage behavior, single particle breakage tests are recommended [71], especially for the prediction of comminution machine performance [72]. Depending on the case of loading, a suitable test method has to be performed. For impact crushers and transportation and handling processes [73], single contact impact tests like drop tests [16], pneumatic guns [74] or tests with rotary impact testers [75, 76] are performed. For most other comminution processes, double contact tests like drop weight, impact load cell [52] or slow compression tests are performed.

The model was originally developed to simulate the degradation of sinter in order to predict the resulting fragment size distribution and fines generation due to transport and storage processes. Thus, single contact impact tests were conducted for this application with a specially developed automated single particle impact tester [77]. The test rig consists of a vibratory bowl feeder to separate the bulk sample, weighing station, air cannon, drop module and integrated fragment analysis by a specially developed vibrating sorter. The high grade of automation allows rapid single particle breakage characterization. A detailed description of the test rig and breakage test results for blast furnace sinter including breakage probability, fragment size distribution, fines production, size-independent relative fines production and characterization with the  $t_n$ -model [78] is provided in [70, 77].

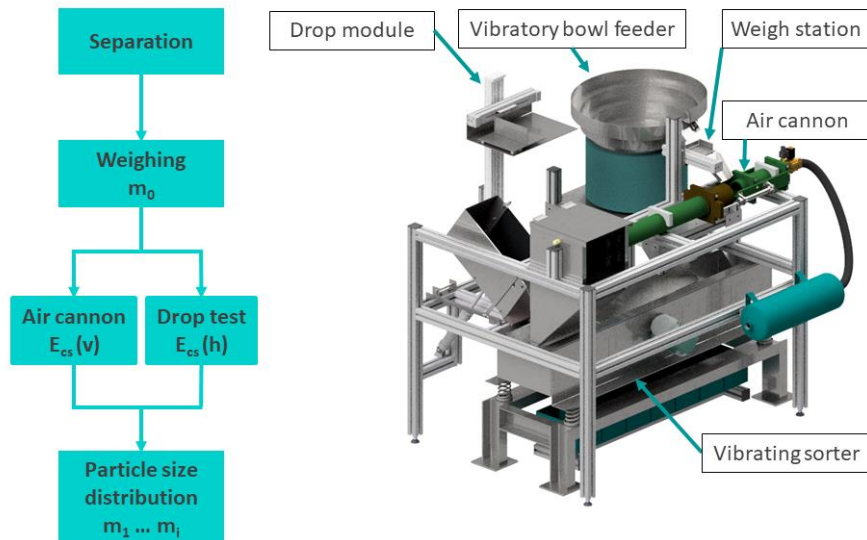


Figure 1: Concept of a highly automated single particle impact tester [77]

### 3. Probabilistic particle replacement with breakage patterns

In order to simulate breakage embedded in DEM with high accuracy in terms of fragment size distribution, in high mass flows and a reasonable computing efficiency, a novel particle breakage model has been developed. The model is based on a probabilistic particle replacement with fragments, which are previously tessellated with the Voronoi algorithm. The model has been developed using the DEM software ThreeParticle with a particle replacement API (Application Programming Interface) in C++. The model uses the recently implemented Voronoi tessellation tool in ThreeParticle. The model was first presented in [67–69] and is described in detail in [70].

#### 3.1. Concept

For Voronoi tessellation, polyhedral particles are required. In this case the initial particles are of spherical shape (resolution of 18 for both rotational axis), but can be of any convex shape. Depending on the stress, initial particles are probabilistically replaced by different particles, similar to [20, 40]. In contrast to [20, 40] and other particle replacement models, the initial particle is replaced by different breakage patterns instead of several smaller spheres. The different breakage patterns have the same mass and volume as the initial particle, which ensures mass and volume constancy. The breakage patterns are predefined and are copies of the initial particle, but have been tessellated with the Voronoi algorithm (see Figure 2). The replacement with previously defined breakage patterns is much more efficient in terms of computational effort than tessellating the particle at the event of breakage, which would mean that the Voronoi algorithm would have to be performed at every event of breakage.

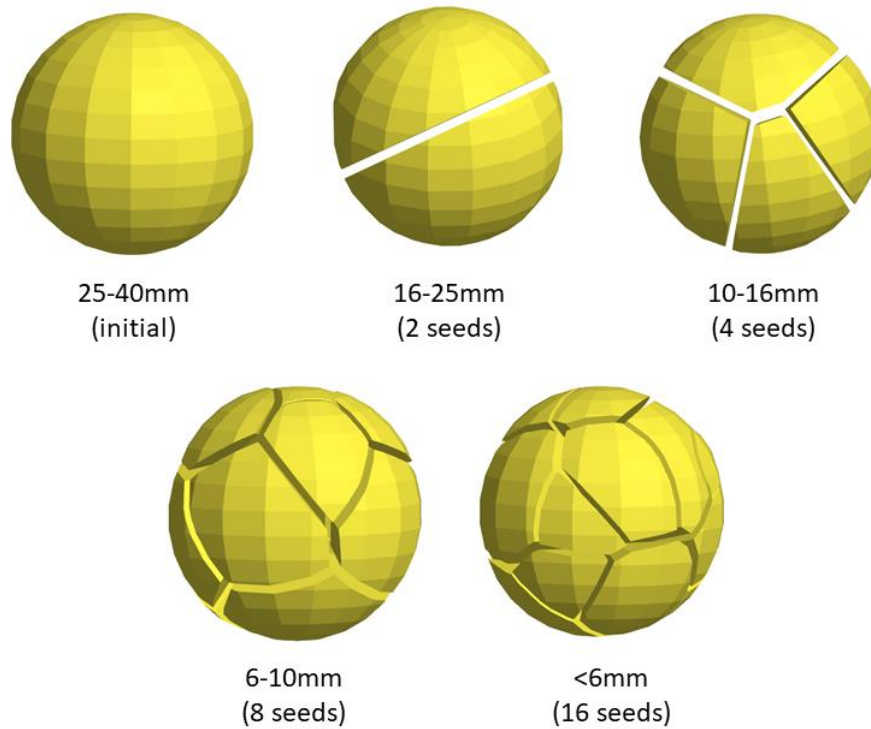


Figure 2: Breakage patterns, which are Voronoi-tessellated polyhedral particles [69]

The Voronoi algorithm is an efficient way to tessellate areas or volumes. For Voronoi-tessellation, randomly distributed points (seeds) are generated. Then the area or volume is divided in the middle of two neighboring seeds. Thus, the average fragment size in this application depends on the number of seeds. The fragments are sharp-edged polyhedral particles and are of random shape. This requires more computing power and usually smaller simulation time steps than with spheres, but ensures mass and volume constancy. No fictive overlaps and temporary damping factors are necessary for the fragments to ensure volume constancy, as needed for a replacement with spheres.

In the here presented example which is shown in Figure 2, size fractions defined by their passing diameter of a conventional screen are defined. It must be stated that due to the random shape of individual fragments, individual fragment masses do not correspond to average particle mass in the respective size fraction. To ensure that the average fragment mass within a breakage pattern approximately corresponds to the average particle mass in the respective size fraction  $m_{fraction}$ , the number of seeds  $s$  can be defined by Equation (1), with  $m_0$  as the initial particle mass.

$$[s] = \frac{m_{fraction}}{m_0} \quad (1)$$

In Figure 2 a particle of 40 mm corresponding to the initial particle size fraction 25-40 mm is depicted. Four different breakage patterns were defined for the different resulting fragment sizes corresponding to the size fractions 16-25, 10-16, 6-10 and <6 mm. To

reduce computing power, fines are represented larger and summarized as 6 mm fragments in this case.

Depending on the stress, the initial particle is completely replaced by fragments of a defined size. The probability for each breakage pattern or resulting fragment size is determined from breakage test results, which were obtained from single particle impact tests with the test rig described in Section 2. A piecewise linear regression is conducted in order to allow simple calculation of the replacement probability at any specific impact energy  $E_{cs}$  using linear interpolation (see Figure 3).

The piecewise linear regression was conducted with Matlab by means of [79] using the least squares method, in which the breakpoints have to be defined by the user (in this case at  $E_{cs} = 14 \text{ J/kg}$  and  $E_{cs} = 49 \text{ J/kg}$ ). The linear equations resulting from this Matlab calculation were then slightly adjusted manually in order to ensure that the sum of all probabilities is 100 at every point. This was achieved by adjusting the gradients that the sum of all gradients in all intervals was 0. These linear equations were then implemented in the particle replacement API. The adjustment is simple and can be performed manually for linear regressions, but could be mathematically complex for other types of regression, which could be more accurate in some cases. For this application a linear regression was considered sufficiently accurate.

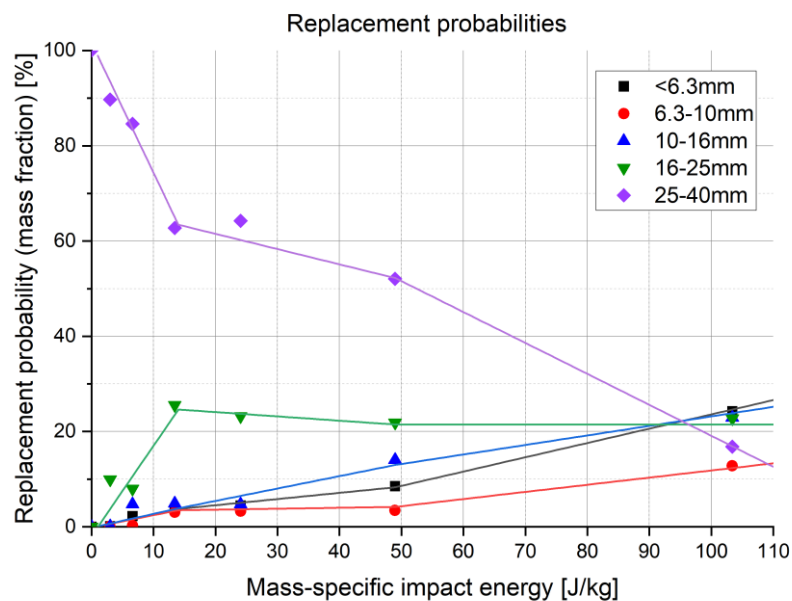


Figure 3: Replacement probabilities for following particles from piecewise linear regression based on breakage test results in [69, 70]

At every compressive force maximum, a corresponding impact velocity and a specific energy is calculated. If the maximum compressive force exceeds a minimum breakage force, a random algorithm is started. At the event of breakage, one of the predefined breakage patterns is determined by the random generator. The probability for each breakage pattern is equivalent to the average mass fraction of the corresponding fragment size after impact at this specific impact energy. When the initial particle size is determined

by the random generator, no replacement occurs. This leads to the correct PSD in the bulk sample, when applied on a high number of particles.

In Figure 4 the breakage model is demonstrated with the impact of sinter particles on a steel plate. As the model is based on probabilities, a number of particles are necessary. The impact of 25 identical initial particles (40 mm in diameter, 47 g) is simulated at different velocities. Figure 4 shows the particles before the impact, moving towards the steel plate. Figure 4b)-d) show the particles after the impact with different velocities, moving away from the steel plate. The color scale represents the particle or fragment mass (0 to 47 g). Shortly after the impact process is completed, the initial particles are replaced by one of the breakage patterns from Figure 2, following the probabilities of Figure 3. The initial 40 mm particles appear red, the 16-25 mm fragments appear green and all smaller fragments (10-16, 6-10, <6 mm) appear blue in this case.

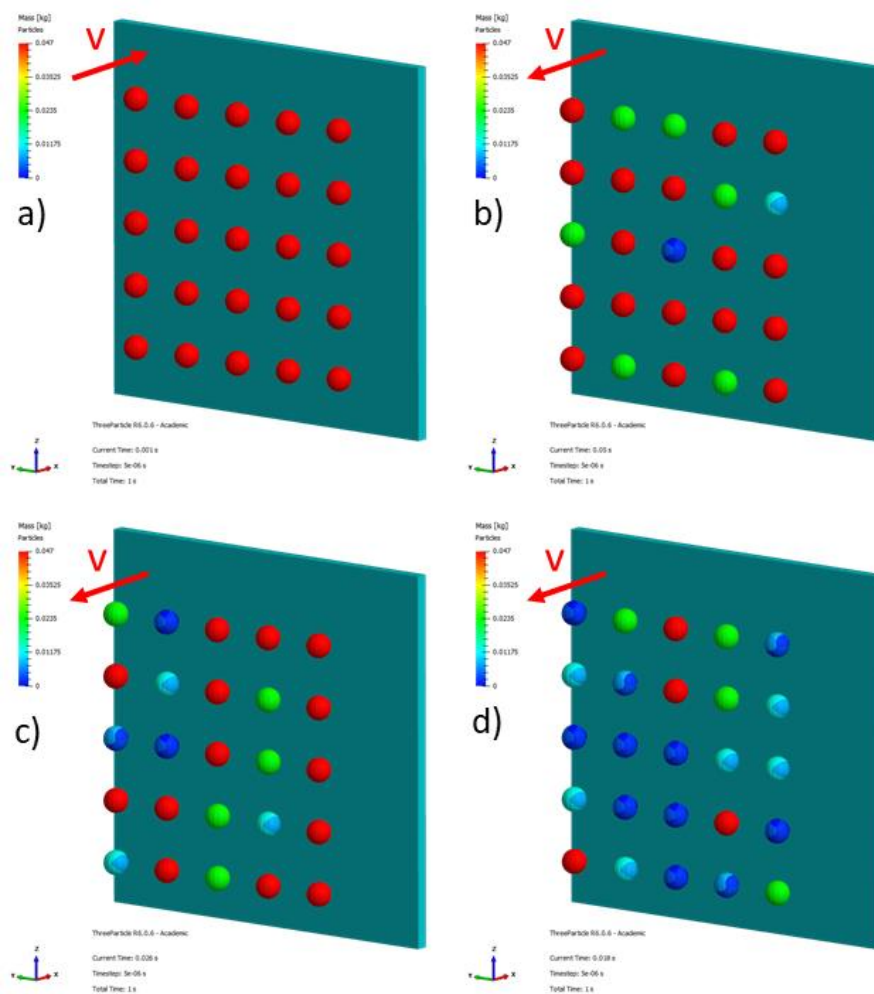


Figure 4: Impact simulation with 25 identical initial particles with  $d=40$  mm and  $m=47$  g a) before impact and after impact with b) 5 m/s (12.5 J/kg) c) 10 m/s (50 J/kg) d) 15 m/s (112.5 J/kg). Color scale represents fragment mass from 0 to 47 g [70]

### 3.2. Correlation between impact velocity and compressive force

The relation between maximum fictive compressive force at an impact and impact velocity is determined by impact simulations with different velocities. In contrast to smooth spheres, the compressive force depends on the alignment for polyhedral particles. For this purpose, the impact simulations were conducted with 1000 particles with random alignment. Then the median value of the maximum compressive forces is used.

Depending on the contact model, different correlations are determined. For polyhedral particles, the Hooke contact model is strongly recommended [70]. If the Hooke model is used, the maximum compressive force  $maxCF$  is linearly dependent on the impact velocity  $v$  following Equation (2). The linear parameter  $a$  was determined for different particles, which differ in shape and mass. If the linear parameter  $a$  is plotted against the particle mass  $m$ , a power trend is noticed (see Figure 5). Another linear parameter  $A$  and the exponent in this power trend depend on simulation parameters. The linear parameter  $a$  is normalized in Figure 5. The linear parameter  $a$  is only dependent on the particle mass  $m$  and is independent of the particle shape. This fact significantly reduces pre-simulation effort to determine the correlation between maximum compressive force  $maxCF$  and impact velocity  $v$ , especially for simulations when the fragments are further breakable (multiple breakage).

$$maxCF = a v \quad (2)$$

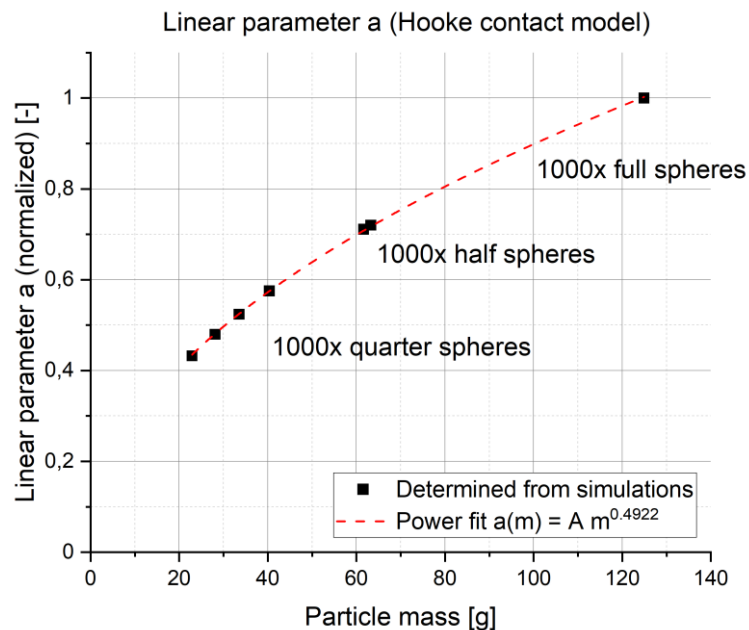


Figure 5: Mass dependency of the linear parameter  $a$  for the correlation between maximum compressive force  $maxCF$  and impact velocity  $v$  with the Hooke contact model following Equation (2).

A detailed comparison of the Hooke and Hertz-Mindlin contact model for impact processes is provided in [70]. The Hertz-Mindlin model could lead to extraordinarily high contact forces in some cases for sharp-edged particles, especially from a certain impact velocity. The Hertz-Mindlin model is suitable for particles with smooth surfaces, which is consistent with statements in [80]. The Hooke model leads to higher and more widely dispersed contact forces than the Hertz-Mindlin model, but does not lead to extraordinary contact forces due to sharp edges. Thus, the Hooke model is more suitable for particles with non-smooth surfaces.

### **3.3. Energy balance**

In contrast to reality, the fragments in Figure 4 do not fly apart in this case. This is due to the fact that the replacement occurs a few time steps after the impact process is completed, which is necessary to avoid unrealistic explosions and a false increase in kinetic energy. If the particle were replaced by smaller fragments during the impact process, which would mean that there was still a certain overlap with the impact surface, this could lead to extraordinarily high overlaps for the small fragments with the impact surface and thus to extraordinarily high reaction forces and explosions.

If the replacement occurs after completion of the impact process, the kinetic energy of the fragments after the breakage is also higher than in reality. The fragments all have a similar velocity after impact, which is only reduced by a damping factor calculated from the coefficient of restitution. Thus, it must be stated that the energy balance is not correct unless the breakage energy is taken into account because the proportion of kinetic energy is too high then.

One method to consider the breakage energy would be to decrease the velocity after the impact by a factor, which could easily be implemented with the API. Therefore, further investigations regarding the breakage energy would be needed. Alternatively, the breakage energy could be estimated by means of the Griffith criterion [81], whereby the breakage energy is proportional to the creation of new surfaces [82] with a given surface energy.

Breakage with fragments flying apart could be visualized with this model by defining an initial overlap among the Voronoi fragments. This could be defined by an offset, which shifts the Voronoi fragments toward or away the center of the particle after tessellation. Figure 2 was created with an explosion offset of +2 mm for better visualization, for example. A negative explosion offset would lead to overlaps among the Voronoi fragments.

### **3.4. Fragment size analysis**

Due to the Voronoi tessellation process, fragments are of random shape and individual fragment sizes vary. In contrast to other breakage models where spheres are used and fragment sizes can be simply determined by diameter, mass or volume, in this model fragment sizes can only be identified by particle names. When particles are defined, every particle is assigned a name containing its size in the first characters, for example. Thus, also for breakage patterns a name corresponding to their size fraction must be assigned. In ThreeParticle the Voronoi fragments resulting from a tessellation are numbered and the name of the initial particle with the suffix `_voronoi_x` is automatically assigned. Here `x` is the number of the fragment, which starts the count at 0. Thus, every fragment can later

be associated with its breakage pattern and categorized into a certain size fraction, independent of its actual size and mass in the simulation. Fragment size analysis can then simply be conducted during post-processing. For this purpose, only the particle masses and names have to be analyzed. Most DEM programs provide tools for this purpose like PSD sensors, for example.

#### 4. Multiple breakage

For longer and complex conveying processes with several damaging events, it can be necessary to generate further breakable fragments. The model presented here allows further breakage of fragments as the generated fragments are also polyhedral particles, which are able to be further tessellated with the Voronoi algorithm.

As individual fragments have different masses and shapes, for each fragment a correlation between impact velocity and compressive force has then to be determined, following the procedure described in Section 3.2 using the Hooke contact model. Evaluations revealed that also for very irregularly shaped and sharp-edged fragments impact simulations with 1000 fragments with random alignment were accurate enough. Maximum compressive force values are more widely dispersed in this case, which reaffirms using the mean value instead of the average value to reduce the impact of outliers.

How often a particle and its resulting fragments can be further broken is described with the breakage level  $L$  in the following. For example, a breakage level of  $L=2$  means that the initial particle for this breakage process is a fragment of a previous breakage process at  $L=1$ .

In Figure 6 multiple breakage for a 50 mm particle of spherical shape is exemplarily shown. At breakage level  $L = 1$  the initial particle is able to break into one of five breakage patterns (40, 25, 16, 10, 6 mm), which are aligned below the initial particle in Figure 6. Breakage by replacement of a breakage pattern tessellated from the same particle is indicated with a black line (Voronoi tessellation). When the 50 mm initial particle breaks into the 40 mm size fraction, two seeds are generated ( $s = 2$ ), which results in two fragments approximately shaped like a half sphere, in this case. The particles in the 40 mm size fraction are then further breakable into the four smaller size fractions at breakage level  $L = 2$ . When the 40 mm size fraction breaks into the 25 mm size fraction, again  $s = 2$  is applied, which splits the half spheres into quarter spheres in this case. The 25 mm size fraction is then further breakable into the three smaller size fractions at breakage level  $L = 3$ . When the 50 mm particle directly breaks into the 25 mm size fraction, it is replaced by a compound particle assembled from its further broken fragments to ensure that the same fragments are generated as from breakage in two steps (via  $L = 1$  and  $L = 2$ ).  $L = 4$  would be further breakage of the 16 mm size fraction in this case, which was not implemented here. As fragment size distribution is determined by names of particles during post-processing (with Matlab routines, for example), the assignment of suitable particle names is very important for this model.

The number of required correlations between impact velocity and maximum compressive force  $c$  also depends on the number of seeds  $s$ , which describes how many fragments are generated at a breakage process. The number of correlations  $c$  can easily exceed to high numbers requiring high calibration and pre-simulation effort. For a

constant number of seeds  $s$  for each breakage level  $L$ , the number of required correlations  $c$  follows Equation (3). However, considering the fact that the linear parameter in Equation (2) is only dependent on the particle mass and independent of the particle shape (see Section 3.2), only a few impact simulations have to be conducted until a trend for the linear parameter  $a$  can be fitted. Then the linear parameter  $a$  can then be easily calculated for each particle with the particle mass  $m$ . Once the linear parameter  $a$  is calculated, the correlation between maximum compressive force  $maxCF$  and impact velocity  $v$  can be calculated with Equation (2).

$$c(s, L) = \begin{cases} 1, & L = 1 \\ \sum_{i=1}^{L-1} s^i + 1, & L > 1 \end{cases} \text{ with } s, L \in \mathbb{N} \quad (3)$$

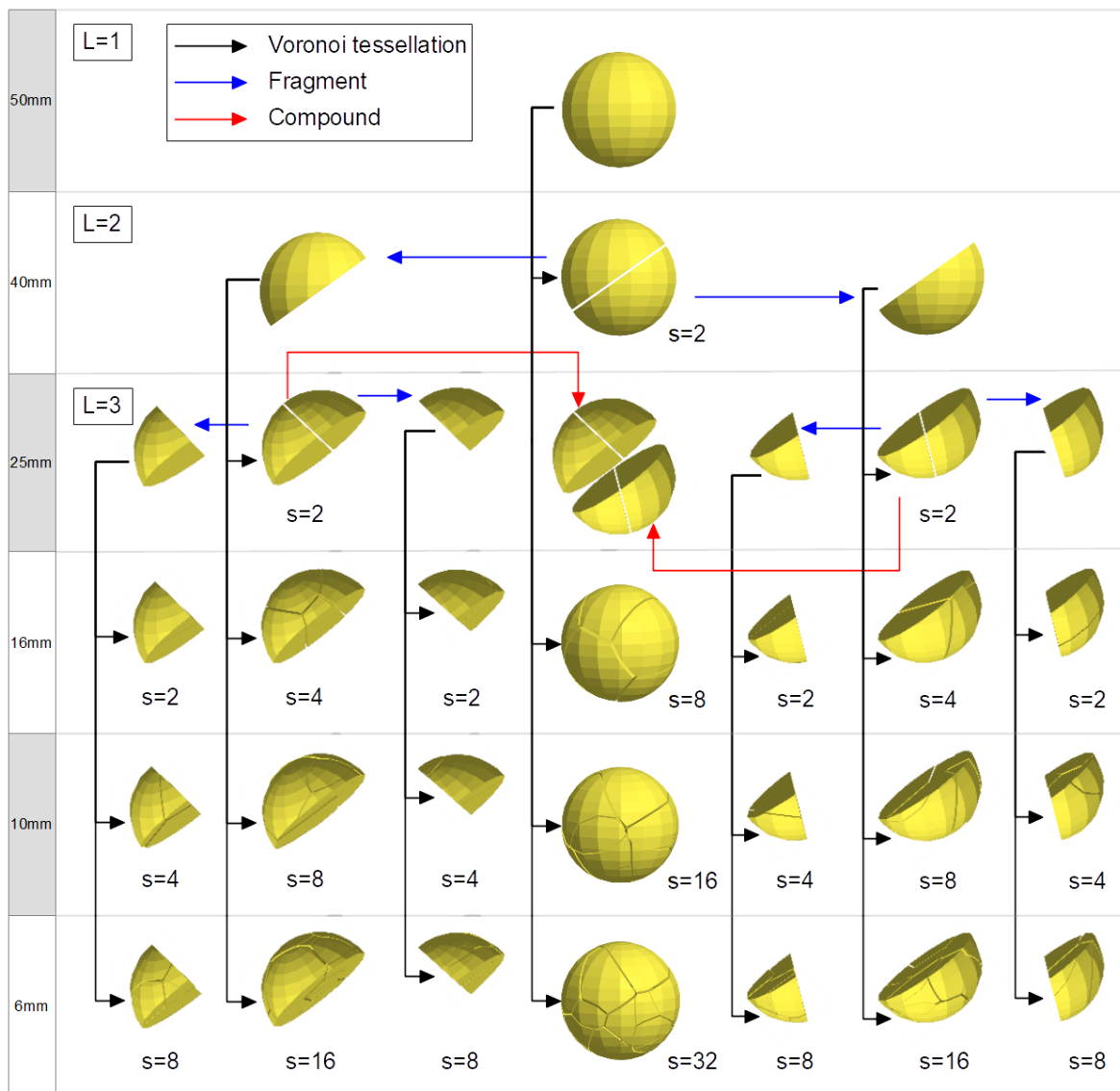


Figure 6: Multiple breakage on 3 breakage levels ( $L=3$ ) [70]

## 5. Computational scheme

The breakage model was developed using ThreeParticle's particle replacement API, which allows the user to extend the simulation software with additional features. Customized functions can be programmed with C++ in the API and will be inserted into the default calculation cycle of the DEM software ThreeParticle.

### 5.1. Custom properties

In ThreeParticle custom properties have been introduced to ease the user's handling of custom variables, which are stored as a common string and can be easily written and read via predefined functions [83]. The custom properties are not deleted when a new simulation cycle starts. In this case, the custom properties are used to take into account the particle history. The custom properties string is assembled from comma-separated values and is converted into a vector of type double with four entries. A description of the custom properties vector is given in Equation (4). In various steps values (type double) are written to and read from the custom properties vector. The first two entries  $customProperties(0,1)$  are updated at the end of the algorithm. This is done by replacing the first value  $customProperties(0)$  by the second  $customProperties(1)$  and by writing the current compressive force into  $customProperties(1)$ .  $CF(t-2)$  describes the compressive force two time steps before.  $CF(t-1)$  is the compressive force one time step before.

$$customProperties = \begin{pmatrix} CF(t-2) \\ CF(t-1) \\ maxCF \\ Breakage\ timer \end{pmatrix} \quad (4)$$

### 5.2. Breakage delay

The breakage delay is necessary to avoid extraordinarily high overlaps and explosions due to almost instant replacement (delayed by one time step) as described in Section 3.3. To implement a breakage delay in the algorithm, a breakage timer is introduced, which is reduced by 1 each time step. The value for the breakage timer or breakage delay is dependent on maximum velocities, particle size and time step. A breakage delay of 50-100 was defined for the simulations presented in this work.

### 5.3. Breakage algorithm

A schematic flow diagram of the algorithm of the model is depicted in Figure 7. All computational procedures before or after this Plugin are summarized as previous or following computation steps of the DEM software in this flow diagram. The computational scheme is executed in every simulation cycle and parallelized for every single particle.

In the first step it is checked if the particle is defined as breakable, by comparison of the particle name with predefined Strings, which correspond to the names of the breakable particles. If not, the whole particle replacement procedure including several if-clauses is skipped for this certain particle, which reduces computational effort.

If the particle is defined as breakable, its custom properties are checked. Generally, when a new particle is created, no custom properties are assigned by default. Thus, the custom properties are empty (no value) for new particles, which leads to errors when

compared with values of the type double. Therefore, the custom properties have to be initialized with 0 values for newly created particles. In the next step the current compressive force  $CF$  on the particle in this time step is compared with a minimum value for breakage. The minimum compressive forces for breakage are calculated with the linear parameter  $a$  from Equation (2) and from minimum mass-specific impact energies for breakage, which are determined from drop tests in [77].

Then it is evaluated if the compressive force  $CF$  peaked in the previous time step ( $t-1$ ). For this purpose, the compressive force values of the two time steps before ( $t-2$ ) and ( $t-1$ ) from `customProperties(0,1)` are compared with the current compressive force in this time step  $CF(t)$  with the condition in Equation (5).

$$CF(t - 2) < CF(t) < CF(t - 1) \quad (5)$$

If a peak for the previous time step ( $t-1$ ) is detected, the maximum compressive force value  $maxCF$  in `customProperties(2)` is set as  $CF(t-1)$  and the breakage timer is set to a defined value (see Section 5.2).

When the breakage timer is 1 and a value is set for the maximum compressive force ( $maxCF \neq 0$ ), the actual particle replacement procedure starts. With the correlation from Equation (2), the impact velocity  $v$  is back-calculated. Then the mass-specific impact energy  $E_{cs}$  is calculated with the impact velocity  $v$  and Equation (6). With a given specific impact energy  $E_{cs}$  the breakage probabilities for each breakage pattern can be interpolated (see Figure 3).

$$E_{cs} = \frac{v^2}{2} \quad (6)$$

Then a random procedure is started. It has to be considered that there is no real randomness in numerics and random generators are actually pseudo-random generators, which deliver the same set of values depending on the seed. Always different sets of values can be obtained when the pseudo-random generator is seeded with a value depending on the absolute time, for example. Most pseudo-random generators deliver normally-distributed values, which is not desired here. Evenly distributed values are needed. For this model the Mersenne Twister MT19937 is used [84], which is an equidistributed uniform pseudo-random generator. A pseudo-random value is generated in the range of 0 to 10000.

With the previously calculated replacement probabilities, intervals in the range of 1 to 10000 are then defined for comparison with the pseudo-random value. Each interval corresponds to a different breakage pattern. Depending on the pseudo-random value, a breakage pattern is selected and the initial particle is replaced. For the following particle, all custom properties are set 0.

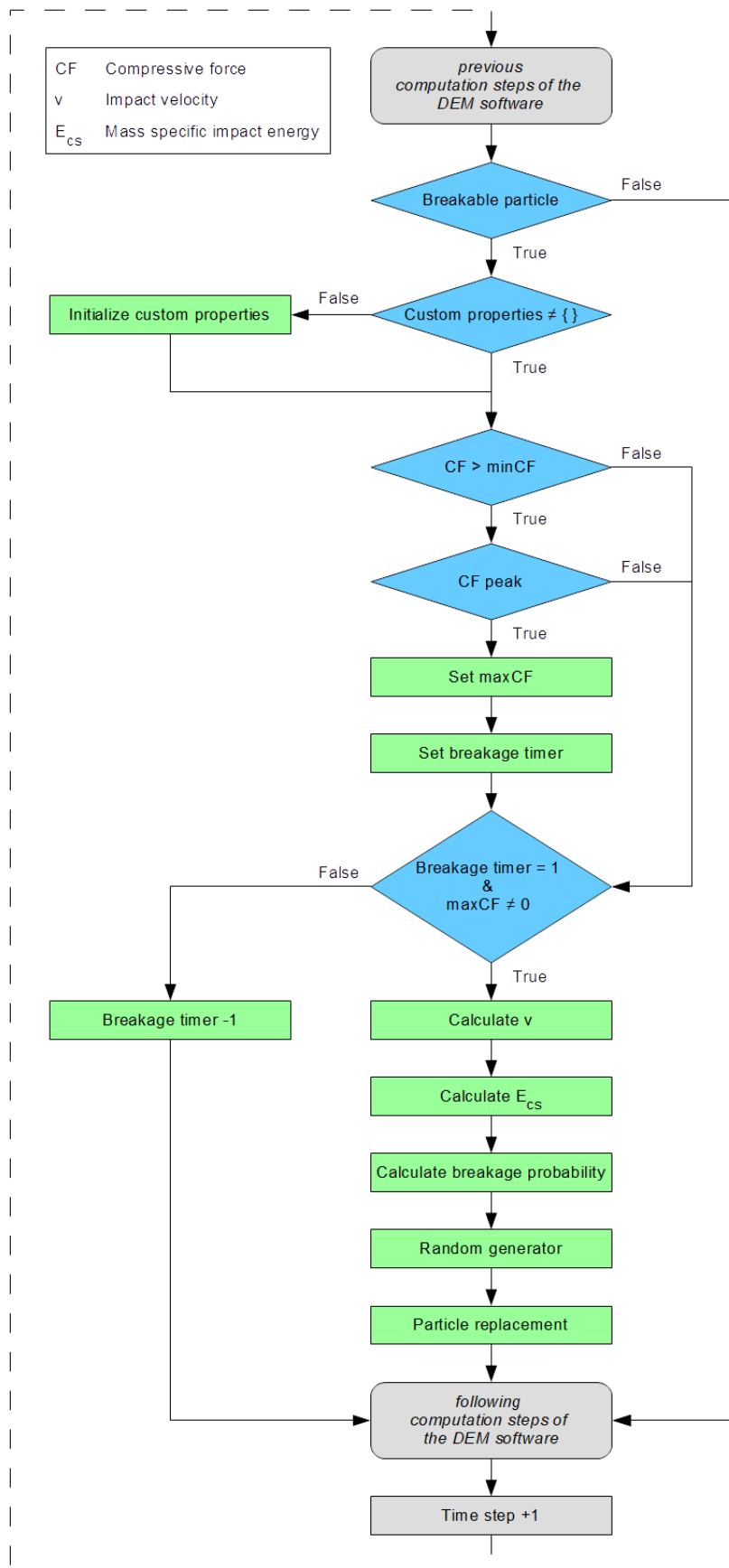


Figure 7: Schematic flow diagram of the breakage algorithm [70]

## 6. Verification and Validation

The novel breakage model was verified and validated with a trial of shatter tests. Furthermore, simulations of conveying trials which are described in [5, 6] including a standard chute and a dynamic transfer system (FlowScape ) were repeated with the novel breakage model and compared with results from the experiments for further validation. The content of this Section was first published in [67–69].

In the shatter tests, a drop apparatus with a quick-opening flap from [85] was used (see Figure 8). The drop apparatus had a drop height of 3.8 m and the bulk material was dropped onto a steel plate at the bottom. The flap was held closed by an electromagnet and was quickly opened by gravity, when triggered. Three tests with 5.7 to 7.5 kg of the size fraction 25-40 mm were conducted. More than four tests would have been desirable, but could not be carried out due to a lack of material. The bulk sample was analyzed before and after the test with the vibrating sorter [77] (see Section 2).

The test was simulated with the DEM software ThreeParticle using the novel breakage model. A time step of  $5 \times 10^{-6}$  s and the parameters listed in Table 1 and Table 2 were used. In Figure 9 the collision of the material with the steel plate at the bottom during the shatter test is depicted at different points in time. The color scale represents the particle or fragment mass (blue=0 g, red=48 g). The particle breakage is clearly visible in the simulation.

Due to the probabilistic approach, accurate simulation results in terms of fragment size distribution require a high amount of particles. An investigation in [69] reveals that a minimum of 3000 particles is required for accurate simulation results in this case. This depends on the breakage probabilities. If the particle amount is below, as for the shatter test (160 particles), the impact has to be simulated several times and the average values for the PSD are used.

The comparison of test and simulation results from shatter tests is shown in Figure 10. The fragment size distribution after the drop is displayed (100% 25-40 mm before the drop). Minimal mass losses are considered as fines (<6.3 mm) due to dust generation and losses during fragment collection. The arithmetic average from the four tests and 25 simulations with standard deviations are depicted. The comparison shows satisfying agreement between test and simulation results.

Material	Density [kg/m <sup>3</sup> ]	Poisson's ratio [-]	Shear modulus [MPa]
Sinter (40 mm)	1455	0.25	10
Steel	7850	0.25	210000

Table 1: Material parameters for shatter test simulations

Interaction	Restitution [-]	Static friction [-]	Rolling friction [-]
Sinter-Sinter	0.75	0.62	0.5
Sinter-Steel	0.43	0.839	0.5

Table 2: Interaction parameters for shatter test simulations [86, 87]

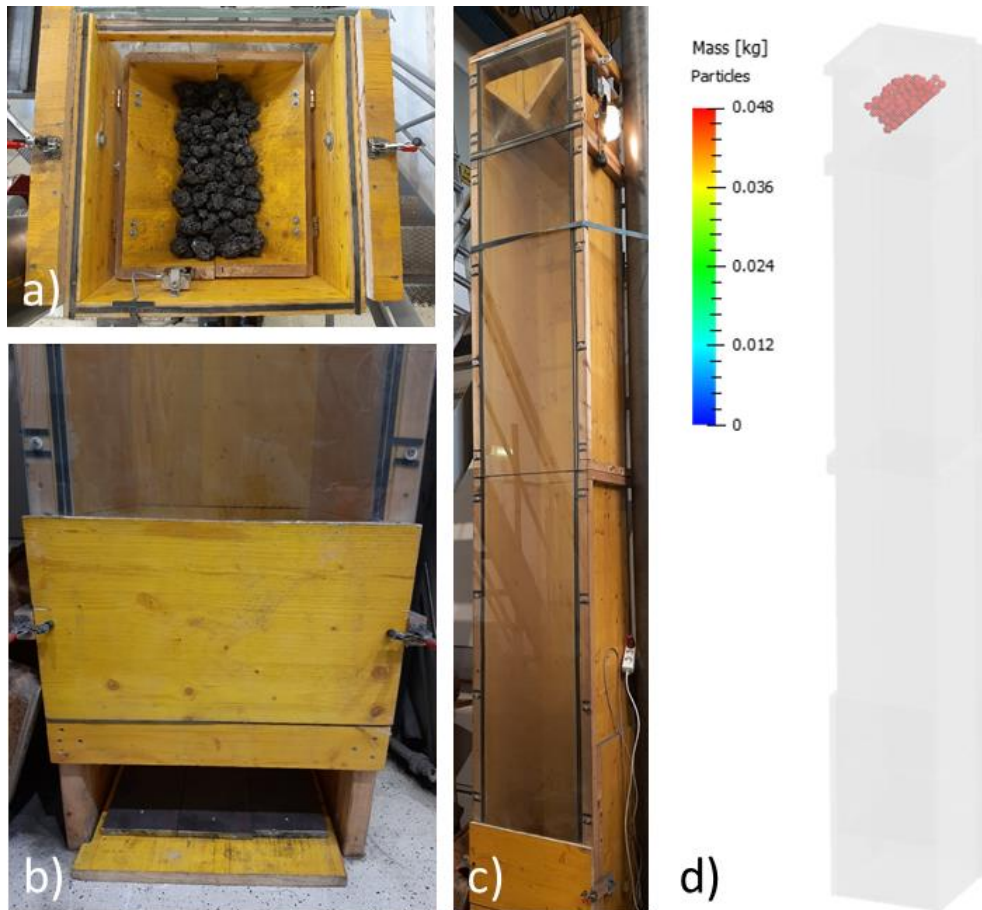


Figure 8: Drop apparatus a) bulk material in quick-opening flap b) steel plate at bottom c) front view d) DE-simulation with ThreeParticle [69]

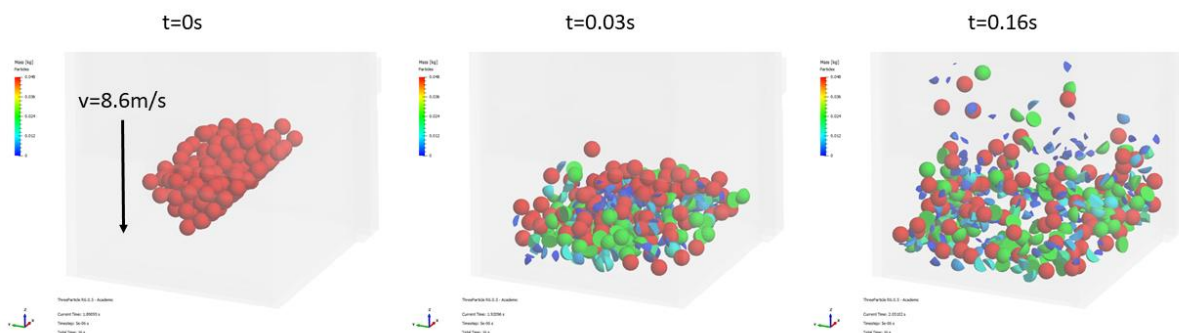


Figure 9: DE-simulation of the shatter test using the novel breakage model showing the collision of the material with the steel plate at different points in time. Color scale represents mass (0-48 g). [69]

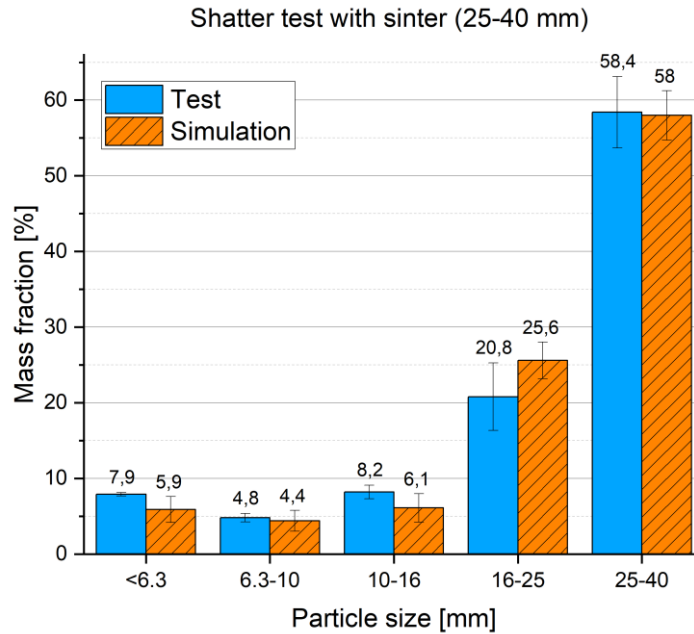


Figure 10: Comparison of test and simulation results from shatter tests [69]

For further validation, bulk material degradation during conveying with two different transfer chutes at the same point was investigated. Originally, this trial was conducted to compare an innovative dynamic transfer system named FlowScape with a standard chute with regard to particle breakage [5, 6, 88]. The dynamic transfer system FlowScape consists of 3 rubber tracks, which are linked with cardanic joints for synchronisation and is driven by a friction wheel on the lower belt conveyor. The FlowScape is patented [89] and described in detail in [90]. A significant reduction of bulk material degradation and in this case 50% less fines generation with the FlowScape was noticed.

The standard chute is a simple cuboid construction with a baffle plate at the rear wall. The drop height for both systems was 1.6 m and belt conveyor speeds were 1.5 m/s. Sinter with 31-50 mm size from a different manufacturer than for the shatter tests was used. With each system 6 tests were conducted and the PSD before and after the transfer point were measured with the vibrating sorter.

The DE-simulations were conducted with ThreeParticle and a time step of  $5 \times 10^{-6}$  s and the parameters listed in Table 3 and Table 4 were used (see Figure 11 and Figure 12). In both simulations 465 kg of sinter was used, which is equivalent to 8319 particles. The color scale represents the particle mass. To represent the size fraction 31.5-50 mm, a particle mix (25, 40 and 50 mm) with the PSD in Table 5, measured in [88], was used. Replacement probabilities in Figure 13 are based on breakage test in [5, 6], where the size fraction 31.5-50 mm with a similar PSD was tested. A detailed description for obtaining the replacement probabilities for a particle mix are provided in [70].

As there are several damaging events, multiple breakage was implemented for this case. All particles and fragments larger than 16 mm were breakable. For particles smaller than 16 mm no breakage was determined in breakage tests at energy levels occurring in these cases [77].

The comparison of test and simulation results is depicted in Figure 14 and Figure 15. The average of each 6 tests is calculated. The increase of mass fractions for each particle size including the standard deviations is depicted. A good agreement of test and simulation results is noticed, especially for fines generation (<6.3mm).

Material	Density [kg/m <sup>3</sup> ]	Poisson's ratio [-]	Shear modulus [MPa]
Sinter (31.5-50 mm)	1908	0.25	10
Steel	7850	0.25	21000
FlowScrape	1400	0.5	7600
Conveyor belt	1400	0.5	7600

Table 3: Material parameters for conveying simulations

Interaction	Restitution [-]	Static friction [-]	Rolling friction [-]
Sinter-Sinter	0.75	0.62	0.5
Sinter-Steel	0.43	0.839	0.5
Sinter-FlowScrape	0.49	0.7	0.5
Sinter-Conveyor belt	0.4	0.7	0.5

Table 4: Interaction parameters for conveying simulations [86, 87]

Size fraction [mm]	Mass fraction (FlowScrape) [%]	Mass fraction (chute) [%]
16-25	15.2	18.2
25-40	74.9	70.3
40-50	9.9	11.5

Table 5: PSD for sinter mix 31.5-50 mm

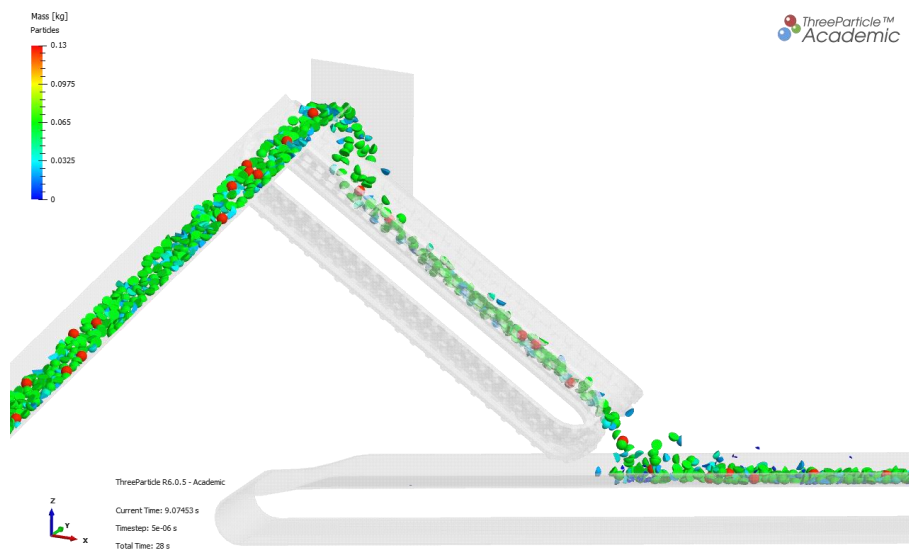


Figure 11: Simulation of the FlowScrape using the novel breakage model with multiple breakage. Color scale represents mass (0 - 0.13 kg) [69]

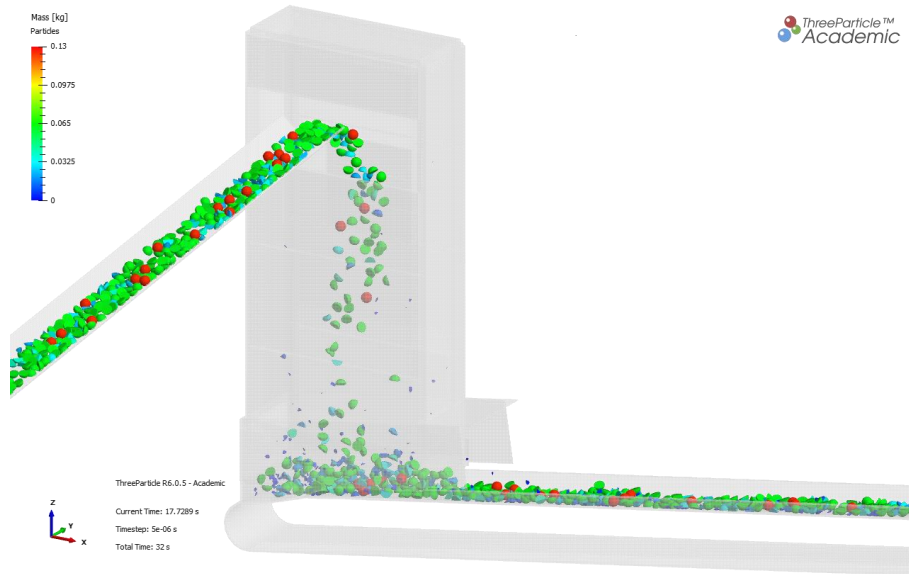


Figure 12: Simulation of the conventional chute using the novel breakage model with multiple breakage. Color scale represents mass (0 - 0.13 kg) [69]

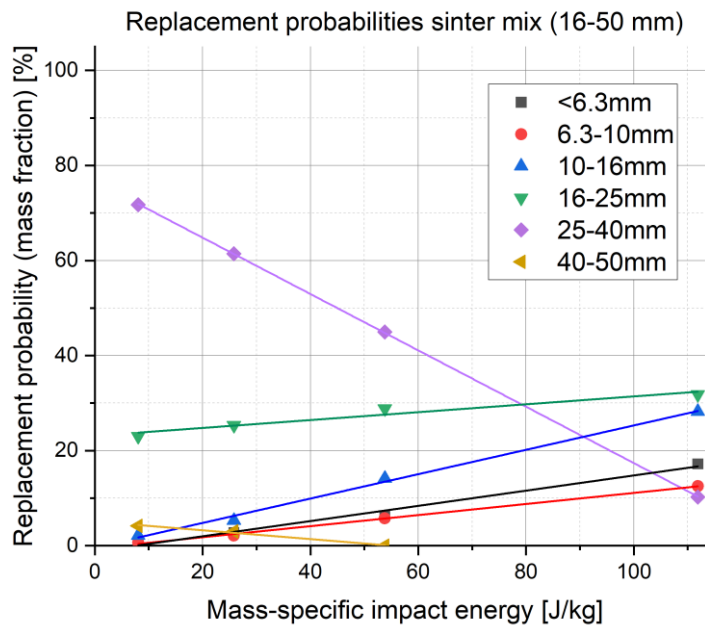


Figure 13: Replacement probabilities for following particles from linear regression for a mix similar to the PSDs in Table 5

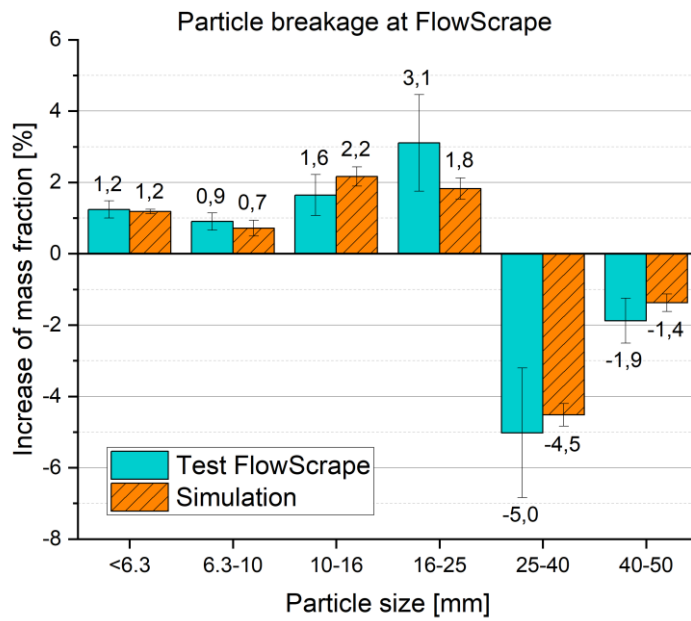


Figure 14: Comparison of test and simulation results: increase of mass fractions due to transfer with the dynamic transfer chute FlowScape [69]

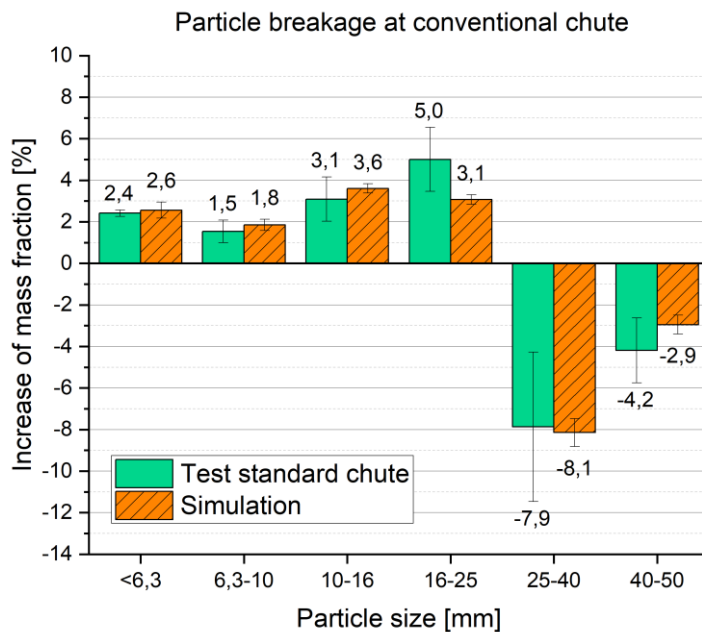


Figure 15: Comparison of test and simulation results: increase of mass fractions due to transfer with the dynamic transfer chute FlowScape [69]

## 7. Summary and conclusion

In order to simulate particle breakage in high mass flows with high accuracy in terms of fragment size distribution and reasonable computing efficiency, a novel breakage model was developed for DEM. The model was developed in ThreeParticle's particle replacement API using C++. The model is based on a probabilistic particle replacement with fragments which were previously tessellated with the Voronoi algorithm. Depending on the stress, the particle is replaced by different breakage patterns. The fragments are sharp-edged and of random shape. Slightly more computing power is necessary than for a replacement with spheres, as in [20] for example. The major advantage is, however, that mass and volume constancy is ensured in this model. Initial particles are polyhedral and can be of any shape.

Replacement probabilities for breakage patterns are obtained from breakage tests. By temporarily logging the damage history of particles, compressive force peaks are detected. After every compressive force peak, a random procedure is conducted to determine if a particle breaks and which breakage pattern is applied. This leads to the correct PSD in the bulk sample if applied to a high amount of particles. It has to be stated that energy balance is not correct in the simulations performed in this work because breakage energy was not taken into account due to missing data. This could be corrected by reducing rebound velocity, when breakage energy was known. For this purpose, further investigations regarding breakage energy are necessary.

The correlation of compressive force and impact velocity can be obtained from impact simulations with a high number of particles. The Hooke contact model is more suitable for sharp-edged particles than the Hertz-Mindlin model. More widely dispersed contact forces are noticed with the Hooke model, but no extraordinarily high forces occur as with the Hertz-Mindlin model, which could lead to explosions. Impact simulations revealed that the compressive force due to an impact is only dependent on the particle mass and that it was independent of the particle shape for the Hooke model.

Multiple breakage or further breakage of fragments can also be implemented with this breakage model. This allows to simulate long and complex conveying processes with several damaging events. An example of multiple breakage on three levels is described. The computational scheme of the model is also described in detail.

The novel breakage model was verified and validated with a trial of shatter tests. The results show satisfying agreement of test and simulation

results. Further validations were conducted with a different batch of sinter from a different manufacturer in a trial of conveying tests with a conventional chute and a dynamic transfer system (FlowScrape) including multiple breakage. Also in these cases, satisfying agreement of test and simulation results were noticed, especially in terms of fines generation.

## 8. Application and Outlook

The breakage model was successfully applied for a solid state material driven turbine used to reduce segregation effects during storage processes [91, 92] or energy recovery [93, 94], which is patented in [95]. Particle breakage due to the turbine was able to be quantified in [70, 92] using the novel breakage model with multiple breakage for a sinter mass flow of 300 t/h. The breakage model is also used to simulate the degradation of Hot Briquetted Iron (HBI) and Direct Reduced Iron (DRI) in two current projects at the Chair of Mining Engineering and Mineral Economics at the University of Leoben.

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