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Research Paper

Application of Breakage Models to Particle Speeds Simulated by Discrete Element Methods

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Abstract. Simulations that calculate the breakage of a given material allow for estimating the particle size produced by comminution equipment. However, conducting these simulations requires a significant amount of time and incurs high computational costs due to the progressive increase in the number of particles during the breakage events. This challenge has prompted the exploration of alternatives, such as employing impact energies present in simulations with solid particles. This study examines the application of two breakage models to particle speeds, analyzing the correlation between the t_{10} value obtained from simulations using solid particles and the value obtained when simulations include breakage. The findings reveal a linear relationship between the results obtained from simulations with breakage and those with solid particles for a rotor that primarily impacts particles during their initial collisions. This relationship holds true for variations in rotor RPM as well as fluctuations in feed flow.

Keywords: DEM, Simulation with Solid Particles, Impact Breakage, Breakage Model, Breakage severity.

1. Introduction

Over the last few years, with the increasing advancements in computational capacity of computer equipment, numerous research works using Discrete Element Method (DEM) simulations have been conducted in various industries that utilize granular materials such as pharmaceuticals, food, and mining [1]. These types of studies aim to investigate particle flow and the effects of interactions between the materials and the equipment involved in industrial transportation or processing. For instance, in the pharmaceutical industry, DEM computational simulations have been employed to assess the powder flow in a lab-scale rotary tablet press with a force feeder [1]. Despite being one of the key machines, it was previously considered a black box. Moreover, the influence of different types of paddle wheels within the die feeder on powder flow during tablet production has been examined, enabling the study of tablet quality in relation to operating conditions such as turret speed, paddle wheel speed, and particle properties [2].

DEM has also been employed to analyze particle collisions during drying processes, specifically in agitated filter drying, by taking into account contact forces, liquid bridge models, capillarity, and viscosity models [3]. These models aim to represent fluid properties such as viscosity, surface tension, and contact angle. Furthermore, DEM can be utilized for simulating powder mixing in the pharmaceutical industry, enabling the evaluation of mixing efficiency [4] and the optimization of mixer designs and operating conditions for non-spherical particle shapes [5]. In the food industry, the main studies are carried out related to the mixing process, for example, simulations of mixing and drying processes [6] using CFD-DEM coupling to model particle shrinkage or the study of the influence of particle size on the shrinkage rate [7]. In addition, the study of particle-liquid mixing in various types of mixers is studied in [8].

DEM simulations have been applied to investigate the comminution stages within the mining sector, with a primary focus on reducing energy consumption, enhancing performance, and minimizing wear of consumable materials. For instance, DEM simulations have examined the impact of material shape on the charge structure within a semi-autogenous mill [9], as well as liner wear [10]. Changes in the operating parameters of semi-autogenous mills and their influence on particle collisions [11], as well as the shape of the charge which can be used as a new way to quantify liner wear [12], have also been analyzed. DEM simulations can also explore particle segregation caused by the shape of liners and lifters bars. It has been observed that multi-profile liners generate varying grinding effects in different sectors with distinct profiles, compared to other sectors with different shape profiles [13]. Additionally, the effect on grinding capacity of varying the profile shape of the lifter bars also affects the power consumption within a ball mill [14].

Due to the significance of the mining industry and the aforementioned reasons, research efforts are primarily focused on crucial stages during ore processing, namely crushing and grinding. At these stages, DEM simulations can be employed to evaluate equipment performance and redesign components, making them extremely useful tools for equipment optimization and design.

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It is worth noting that the primary function of the crushing and grinding comminution stages is to reduce the size of mineral ores in order to liberate valuable minerals, which can also be simulated using DEM. However, simulations involving particle breakage with discrete element methods are computationally intensive and time-consuming. Therefore, in cases where high-performance workstations are not available, alternative approaches need to be explored. This paper addresses one such possible solutions, which involves estimating the breakage results using the t_{10} value (defined as the cumulative mass percentage of the product passing 1/10th of the initial feed size) which represents the severity of breakage and is obtained using a breakage model. This value quantifies the percentage of mass in broken particles consisting of fragments smaller than one tenth of the original particle size, relative to the total mass (mass of the particle before the breakage event).

This study aims to estimate the t_{10} value using particle speeds obtained from simulations of unbroken solid particles. Such simulations require less time and computational resources, making them suitable for scenarios involving multiple simulations and requiring faster results. To achieve this objective, the proposed approach involves applying breakage models to cases where particle breakage occurs in a single event, which is typical in equipment that employs impact as the breakage mechanism. By utilizing simulations without breakage, the speeds of all particles at each time step are obtained. After a contact identification process, the breakage models are applied during post-processing stages using an in-house code. The obtained results compared with simulations that include breakage via DEM simulation, and the possibility of applying this method to estimate the t_{10} value for a double rotor equipment is analyzed.

2. Methodology

Impact breakage occurs when high-velocity stresses are applied, leading to a rapid exchange of energy between the impacting elements. Several authors have proposed models to assess the probability of breakage for specific materials, which depends on the stress conditions applied by comminution or testing equipment. These breakage models can be incorporated into DEM simulations to obtain the selection function, also known as the probability of breakage, for a given comminution equipment. However, implementing these breakage models comes with high computational costs and long processing times. These challenges make it difficult to use DEM simulations in the design stages of comminution equipment, especially when seeking parametric design and lacking sufficient computational power. This is because the DEM simulation algorithm with breakage not only calculates impacts and the resulting forces but also determines the amount of broken material and the distribution of progeny particles. Additionally, the generation of particles after successive breakage events in DEM simulations increases the number of particles, prolonging simulation time and requiring more computational resources. Conversely, DEM simulations of solid particles, even when simulating a large number of particles, are usually computationally less demanding.

To implement DEM algorithms that incorporate breakage, three relationships are necessary, as indicated by Morrison [15]:

- The selection function (Probability of breakage S).
- The breakage severity represented by the t_{10} value.
- The size distribution of the progeny particles.

The last one can be obtained using the relationship between the t_n values and the t_{10} value provided by Narayanan & Whiten [16]. The definition of t_n values and their relationship with the t_{10} value are illustrated in Fig. 1 and Fig. 2, respectively. t_n values are defined as the cumulative mass percentage of the product passing 1/nth of the initial feed size.

In this study, Vogel & Peukert's model [17] and Tavares's model [18] were utilized to implement them into the speeds of solid particles obtained from DEM simulations without breakage. The results obtained from these simulations were then compared with those obtained from DEM simulations that incorporated continuous breakage using Tavares's model. This comparison was carried out specifically for impact equipment that primarily induces breakage during the initial impact. The focus was on analyzing the relationship between the t_{10} values obtained from simulations with breakage and those obtained by applying the breakage models to the particle speeds.

To apply the impact breakage model, non-breaking simulations were conducted for both individual particles and particle flows within complete equipment. Solid limestone particles were used for these simulations, performed using the commercial software ROCKY DEM. Subsequently, an algorithm was employed to analyze the particle speeds, identify impacts by examining changes in velocity, make necessary corrections and replacements of velocity values when relative velocity is required, and apply the respective breakage model to determine the t_{10} value associated with the obtained speeds. The results obtained from this approach were compared with the results obtained from DEM simulations that included continuous breakage through the application of Tavares's model.

The objective of the procedure presented in this paper is to establish the relationship between the outcomes of simulations with breakage and those obtained by applying the breakage models to the speeds derived from simulations involving solid particles.

3. Breakage Models

The simulation software Rocky DEM offers two breakage models for instantaneous breakage simulations: the Abt-10 model and the Tavares model. In this research, we use the Vogel & Peukert's model [17] and the Tavares's model [18] for our analysis. While the Vogel & Peukert's model differs slightly from the model present in the software, it exhibits similar behavior. On the other hand, the Tavares model is identical in both the software and this article.

These two models are studied to implement DEM simulations that incorporate breakage solely during the initial breakage events. The objective is to determine which model is more suitable for representing the total breakage that would be obtained if the simulation were conducted with continuous application of the breakage model. This approach aims to achieve significant results using modest computational resources and reduce simulation time. The breakage models are described below, along with their respective equations, ranging from Eq. (1) to Eq. (15).

3.1. Vogel & Peukert's Model

The first model to be studied was introduced by Vogel & Peukert's model [17] which was developed by coupling dimensional analysis and fracture mechanics. This model is characterized by the simplicity of its mathematical equation and by explicitly showing the relationship between material parameters and the influence of particle size during breakage.

According to this model, the breakage probability S can be calculated as follows:

$$S = 1 - \exp\left[-f_{MAT} \cdot x \cdot k \cdot \left(W_{m,\mathrm{kin}} - W_{m.\min}\right)\right] \tag{1}$$

In this equation f_{MAT} is a material parameter, x is the particle size, k is the number of successive impacts (up to 3), and $W_{m,\mathrm{kin}} - W_{m.\min}$ represents the energy available to break. In the case of successive impacts, this model implies that each of these impacts occurs at the same specific energy, which in practice is not the case, so Morrison et al. [15] propose a modification to this model applied to successive impacts with different specific input energies:

$$S = 1 - \exp\left[-b' \cdot \sum_{i=1}^{n} [E_i - E_0]\right] \tag{2}$$

In this expression, i represents the i^{th} impact event out of a total of n impacts each of different magnitude, while $E_i - E_0$ represents the energy available to break as long as E_i is greater than E_0 otherwise it won't provide energy that causes breakage, and b' is the material parameter that includes the effect of particle size and is equal to $f_{MAT} \cdot x$.

The breakage severity represented by the value of t_{10} can be calculated according to Morrison et al. [15] by the following equation:

$$t_{10} = M\left(1 - \exp\left[-b' \cdot \sum_{i=1}^{n} [E_i - E_0]\right]\right) \tag{3}$$

In this equation, M represents the maximum t_{10} value whereas the latter represents the fraction from size distribution less than 1/10th the original size.

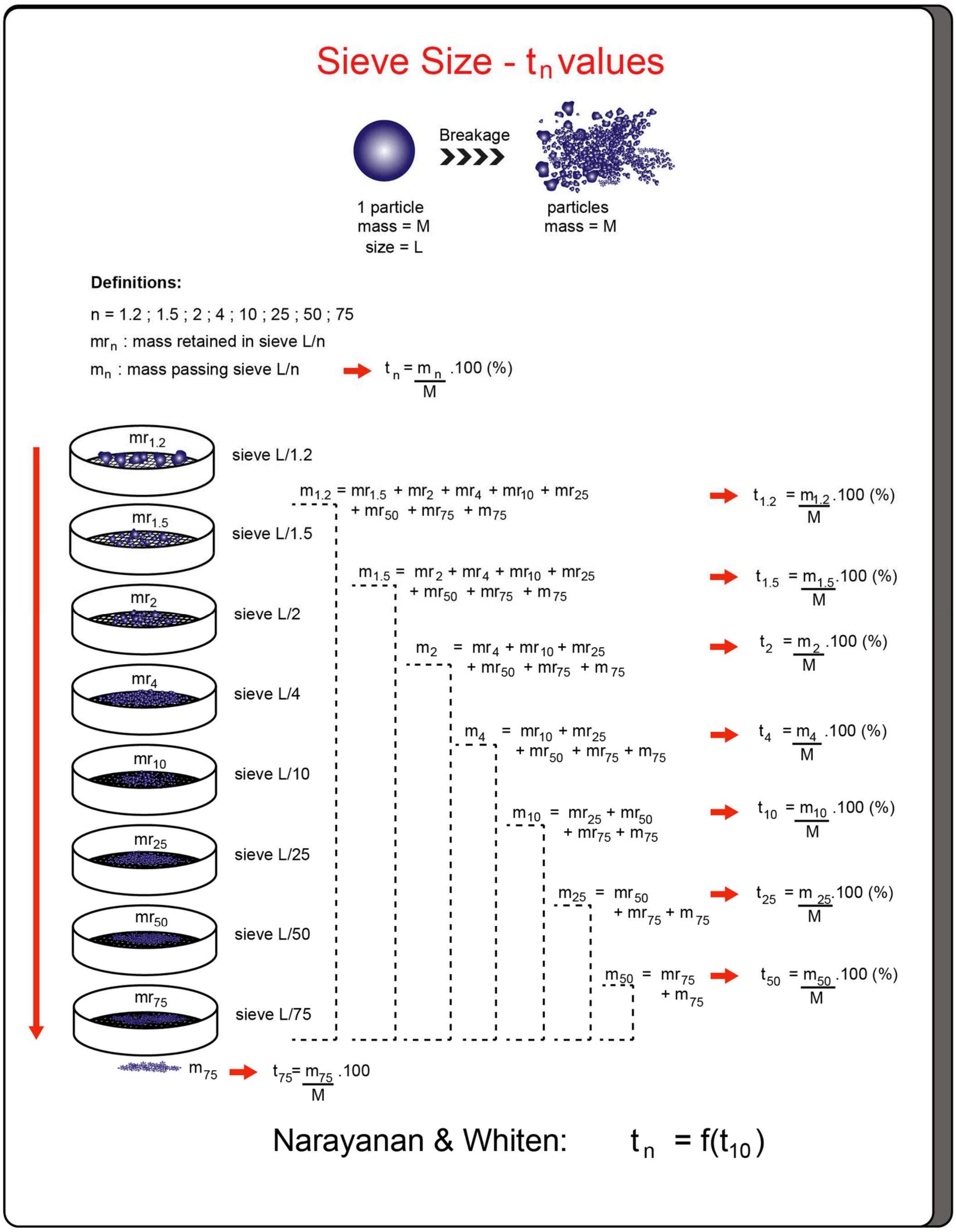

Fig. 1. Definition of t_n values.

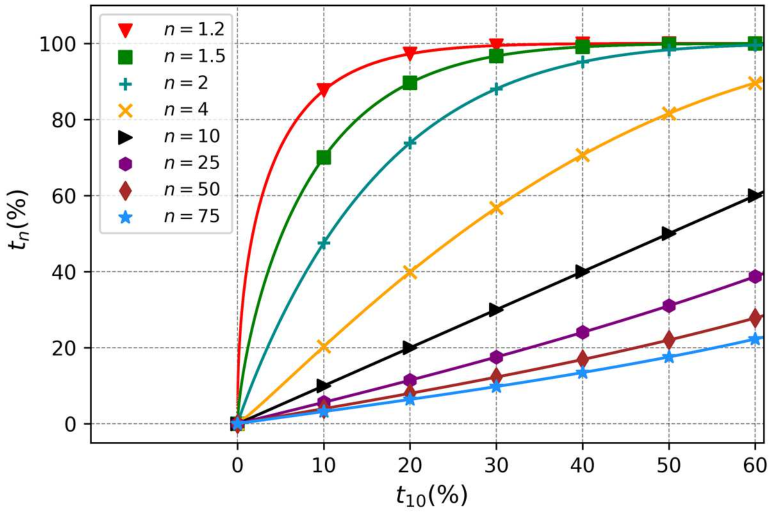

Fig. 2. Relation of t_{10} values with t_n family curves.

In this case, only the probability of breakage resulting from a single impact of particles against the rotor was considered. Therefore, the t_{10} was evaluated using the equation provided by Shi & Kojovic [19]:

$$t_{10} = M\left(1 - \exp\left[-f_{MAT} \cdot x \cdot k \cdot (E_{CS} - E_{m.\min})\right]\right) \tag{4}$$

This expression has the advantage that it can use the weight drop test databases using the following relation provided by the authors:

$$A \cdot b = 3600 \cdot M \cdot f_{MAT} \cdot x \tag{5}$$

With the calculation of t_{10}, the distribution of progeny particle sizes can be estimated.

3.2. Tavares's Model

The second model analyzed is the one developed by Tavares which states that the probability of a particle breaking is adequately represented by a log-normal distribution [18]. Furthermore, this model uses an additional parameter γ that allows quantifying the accumulated damage in particles that receive low energy impacts. For the case where particles impact against a hard target or are simply thrown due to the action of gravity, the specific impact energy can be calculated by the following equation:

$$E_k = \frac{v_0^2}{2} \tag{6}$$

This model states that the breakage energies of particles can be described by the log-normal distribution which is suitable for describing the breakage energies of particles for different materials of different shapes. The cumulative distribution function [18] is given by:

$$P(E_k) = \frac{1}{2}\left[1 + erf\left(\frac{\ln(E^*) - \ln(E_{50})}{\sqrt{2\sigma^2}}\right)\right] \tag{7}$$

where E_k is the specific impact energy and $P(E_k)$ is the probability of a particle breaking when that energy is applied to it. The value of E^* makes the cumulative distribution function into a log-normal upper truncated distribution [18]. This value is calculated as follows:

$$E^* = \frac{E_{\max} \cdot E_k}{E_{\max} - E_k} \tag{8}$$

In the above expression $E_{\max}$, E_{50}, σ^2 are model parameters that represent the maximum value of the energy, the median, and the variance of the distribution, respectively.

In turn, the influence of particle size on the energy required to cause breakage is observed in the relationship between model parameters and the median value E_{50}, which depends on the particle size d_j, a characteristic size of the material microstructure d_0 and the residual particle breakage energy E_∞ for large particles [18]. This relationship is given by:

$$E_{50} = E_\infty\left[1 + \left(\frac{d_0}{d_j}\right)^{\varphi}\right] \tag{9}$$

By calculating the probability of breakage using the log-normal distribution, the stress-causing energy can be related to the value of t_{10} by the following relationship [18]:

$$t_{10} = M\left(1 - \exp\left[-\frac{b' \cdot E_k}{E_{50b}}\right]\right) \tag{10}$$

where M and b' are model parameters, which are fitted from experimental data. In cases where sufficient energy is applied to cause breakage on a first impact the value, E_{50b} is equal to E_{50}. In cases where the stresses are of a magnitude less than that needed to cause breakage, E_{50b} will be the median fracture energy of the particles that have broken and is related to E_{50} by the following expression [18]:

$$E_{50b} = E_{50} \cdot \exp\left[\sqrt{2}\sigma \cdot erf^{-1}\left(P_0\left(E_k\right) - 1\right)\right] \tag{11}$$

In cases where the breakage event occurs after multiple impacts, the specific fracture energy is modified after each impact event that does not cause breakage and is reduced by the following equation [18]:

$$E_n = E_{n-1} \cdot \left(1 - D_n\right) \tag{12}$$

where E_n is the specific fracture energy at the calculation time step while E_{n-1} is the specific fracture energy of the previous time step. The damage received by the particle with an impact specific energy less than the fracture specific energy is presented by the quantity D_n^*, which can be calculated by the implicit formula [18]:

$$D_n^* = \left[\frac{2\gamma}{\left(2\gamma - 5D_n^* + 5\right)} \times \frac{E_{k,n}}{E_{n-1}}\right]^{2\gamma/5} \tag{13}$$

where γ is the damage accumulation parameter, $E_{k,n}$ is the specific impact energy at the calculation time step while E_{n-1} is the specific fracture energy at the previous time step.

By using this damage accumulation parameter γ one can model the reduction of particle impact resistance after having received damage from low energy impacts.

4. Solid and Breakage Simulations

Two types of simulations are conducted in this study. The first type involves solid particles without the application of a breakage model, while the second type utilizes the Tavares model implemented in the commercial software Rocky DEM to continuously apply breakage. A collection of quasi-spherical polyhedral-shaped limestone particles with a size of 10 mm is used (Fig. 3). This choice is made to obtain results that are closer to those that would be obtained if spherical particles were simulated, since the software does not support breakage for spherical particles. The quasi-spherical shape is advantageous for two main reasons. Firstly, it closely resembles spherical particles, which require minimal computational resources and execution time in simulations. Additionally, this research article aims to analyze the potential application of breakage models in post-processing stages to the particle speeds obtained from simulations with spherical particles that do not incorporate breakage in their configuration. The second advantage relates to the reduced variability of results obtained from simulations using spherical particles, compared to simulations involving non-spherical particles without symmetry or sphericity.

However, it is important to acknowledge that particle shape influences the outcomes of DEM simulations, as observed in the charge shape of a SAG mill [12]. Thus, the applicability of the methodology presented in this article to simulations involving particles with shapes other than spherical or quasi-spherical should be examined in future studies. The simulations are conducted using an impact rotor, and four scenarios are investigated: (1) varying the rotor speed for a single particle to obtain different impact speeds, (2) varying the rotor speed for a particle flow, (3) maintaining a constant rotor RPM while varying the feed flow, and (4) varying the RPM of the rotors in a double rotor impactor.

4.1. Solid Simulations without Breakage

The simulations are conducted using the commercial software Rocky DEM, which calculates contact forces between particles and tracks their positions and speeds. However, the software does not incorporate breakage calculations when impacts occur (Fig. 4). Consequently, simulations are performed without considering breakage, allowing for faster and computationally fewer demanding results in terms of particle speeds. The challenges in design a comminution machine using faster computation simulation are the main reason why the present research activities and computational simulation are performed. The aim is to obtained a faster computational support for designers at the earliest design stage.

In the first scenario, a rotor and a single particle are used, and the rotor RPM is varied from 100 RPM to 1800 RPM. A total of nineteen rotor speed values are simulated, and this process is repeated five times for each RPM. This scenario aims to investigate the influence of varying impact energy on an individual limestone particle. It should be noted that DEM simulations are not deterministic, meaning that in each repetition of the same simulation, both with and without breakage, the particles have different values of specific fracture energy randomly assigned by the software. By varying the RPM, it is intended to determine whether it is feasible to apply breakage models in post-processing stages when only one particle is present.

In the second scenario, a rotor and a particle flow are used, and a constant feed flow of 100 T/h is maintained. The rotor RPM is varied from 400 RPM to 1800 RPM, with a total of fifteen rotor speed values simulated and five repetitions for each RPM. This scenario investigates the impact of varying impact energy on a constant set of particles. In this case, the randomness in assigning specific fracture energy to the particles is not a significant factor since, on average, the particles have similar specific fracture energies in all repetitions of the simulation.

Fig. 3. Quasi-spherical particle used in DEM simulations.

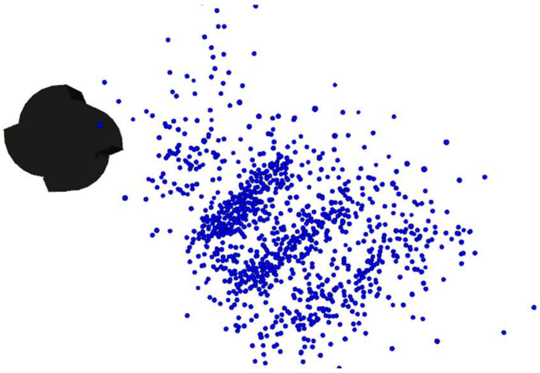

Fig. 4. Particle flow and impact rotor in simulation without breakage.

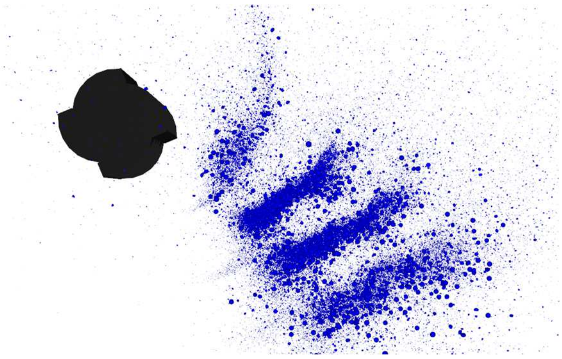

Fig. 5. Particle flow and impact rotor in simulation with breakage.

The third scenario involves a single rotor and a particle flow, with a constant RPM of 1800 RPM and varying feed flow rates from 60 T/h to 400 T/h. Fifteen feed flow values are simulated, and the process is repeated five times for each feed flow value. This scenario analyzes the influence of the number of particles impacting the rotor on the obtained results. As the number of particles increases, the importance of randomness decreases.

In the fourth scenario, a scaled prototype of a dual rotor particle flow impactor is used. A constant feed flow rate of 36 T/h is maintained, and the rotor speed is varied from 800 RPM to 1800 RPM, with six rotor speed values simulated. This scenario aims to explore the application of the proposed method on real equipment that may have more than one impact rotor. The objective is to assess the feasibility of employing a similar procedure, with appropriate adjustments, in cases involving multiple impacts per particle.

The simulation configurations in the scenarios are similar, except for the fourth scenario, where the complete equipment is employed, and only the parameter relevant to each scenario is varied. The position, velocity, and size of each particle are recorded for all time steps in each simulation and it is further processed to apply the breakage models to the particle speeds obtained from these simulations.

4.2. Simulations with Breakage

The simulations that include breakage are also performed using the commercial software Rocky DEM following the same procedure used in the simulations without breakage; in these simulations, the breakage process implemented in the software is applied using the Tavares's model (Fig. 5). To perform this type of simulations, the limestone parameters for the Tavares' model were used, which are shown in Table 1 and are taken from [20]. The limestone material used in the simulations was chosen due to two main factors: the first one is related to the low resistance to breakage that this material presents while the second one is due to the ease of obtaining in the literature the parameters of the breakage model for this material. In this way it is not necessary to obtain the single particle breakage data and estimate the parameters using procedures detailed in [21] and [18]. This simple selection of the material along with its parameters can be done due to the nature of the present investigation where we want to compare the results of simulations that include breakage with the results obtained from applying the breakage models in the post-processing stages for which we use the same parameters of the limestone material for both types of simulations. However, the results obtained in the present investigation should be subsequently verified using different materials with their respective parameters of the breakage model.

Table 1. Limestone parameters for Tavares's breakage model.

Breakage model parameters [20]	
Parameters	Limestone
γ	5.4
σ^2	0.642
A	53.3
b'	0.033
E_∞ (J/kg)	7
d_0 (mm)	100
φ	0.8
E_{max} / E_{50}	4
Density (kg/m^3)	2710
Young's Modulus (N/m^2)	1x10^8

The limestone material parameters necessary for the application of the Tavares breakage model both in the application via software and in the manual application in post-processing stages are: γ the damage accumulation coefficient , which is an index that quantifies whether the damage occurs gradually or suddenly; σ^2 the variance of the distribution; the parameters A and b' resulting from the data fit; E_∞ represents the residual particle fracture energy of the largest material size; d_0 is a characteristic size of the material microstructure; φ is a constant of the model; E_{max} / E_{50} is a relationship between two parameters of the model; density, Young's Modulus.

t_{10} values are obtained directly in this type of simulation since the product of applying the model continuously is the complete distribution of the product particle sizes. These results are compared with those obtained by applying the breakage model to the particles' speeds.

5. Application of the Breakage Model to Particle Speeds in Simulations with Solid Particles

The application of the Vogel & Peukert's model [17] and Tavares breakage model [18] using the velocities obtained from the solid particle simulations is performed by an algorithm, which receives the position, velocity and size data of all solid particles at all time steps.

First, the impacts produced are detected by analyzing the particle velocity changes. Then, the specific fracture energies are established depending on the model in question. In the application of the models, relative impact velocities are used, and velocity corrections are made when a particle-particle impact occurs. However, when a particle-rotor impact occurs, the relative velocities of the particles with respect to the rotor are very close to the rotor velocities at the time of impact. For this reason, it isn't necessary to correct the particle velocities when they impact the rotor.

It should be noted that the establishment of the specific fracture energy is defined whether or not there is breakage when an impact occurs and only if this occurs, t_{10} is calculated for the particle analyzed. The general procedure for applying the models to velocities is shown in the flow diagram in Fig. 6.

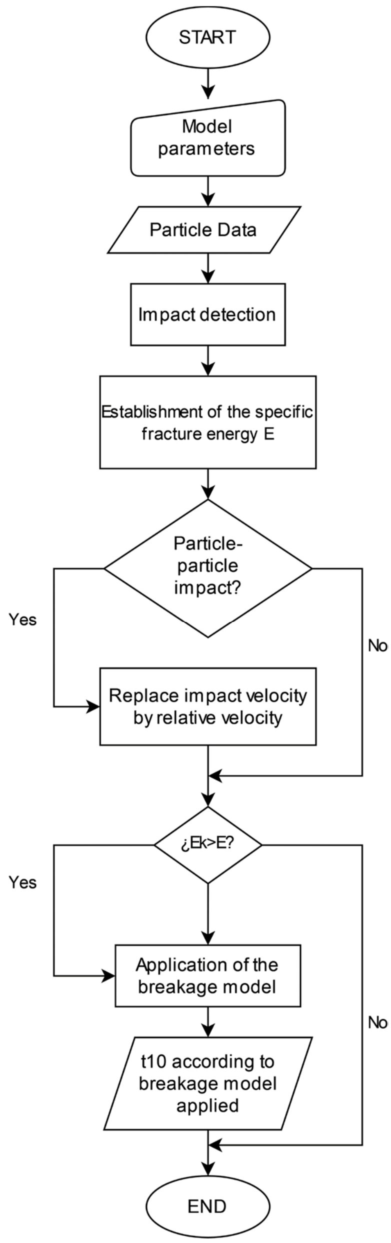

Fig. 6. Process flow diagram of applying breakage models to particle kinematics.

6. Results

Results were obtained for both types of simulations with and without breakage. It was not necessary to correct the chosen parameters of the breakage model for the limestone material since the purpose of this publication is to apply the breakage models in post-processing stages for simulations that do not include these calculations in their configuration. For this reason, the validation of the results obtained from the application of the models to the particle speeds of simulations without breakage is obtained from the results of probability and severity of breakage of simulations that do include this event via software which are highly demanding and computationally expensive.

Both Vogel & Peukert's model [17] and Tavares breakage model [18] are applied to calculate the probability of breakage and the t_{10} for the speeds obtained from the simulations with solid particles. For this purpose, the specific fracture energies of the particles present in the simulations were established according to the applied model taking into account that for the Vogel & Peukert's model the impact energies must exceed threshold energy to produce breakage, while for the Tavares's model, the impact energies must exceed the random specific fracture energies that follow the log-normal upper truncated distribution. In the case of Vogel & Peukert's model this value quantifying the particle resistance to breakage is given by the threshold energy, which is material and particle size dependent whereas, for Tavares' model, the specific fracture energy is set randomly following the algorithm [22]:

Step 1. A random value between 0 and 1 is generated for each particle.

Step 2. A specific energy value is assigned to each particle corresponding to the value between 0 and 1 that was assigned as the probability of breakage to that particle considering the log-normal or log-normal upper truncated distribution (Fig. 7).

Results are obtained for the four scenarios:

1) Single particle and a rotor with rotor RPM variation.
2) A particle flow and a rotor with variation of rotor RPM.
3) A particle flow and a rotor with feed rate variation.
4) A particle flow in a double rotor impact equipment with variation of the RPM of both rotors.

Results are obtained for the three scenarios: a single particle with rotor RPM variation, a particle flow with rotor RPM variation, and a particle flow with feed rate variation.

Finally, complete impact equipment with a double rotor is analyzed in order to study the estimation of t_{10} values by applying the breakage models to the particle speeds obtained from simulations with solid particles. In this last case, it is also sought to estimate the combined effect of both rotors by estimating the effect of each one of them separately using the procedure proposed in this work.

On the other hand, the t_{10} values for the simulations with breakage in all scenarios are obtained directly from each simulation.

6.1. Single Particle Impact into One Rotor with RPM Variation

In the case of single particle simulations, the breakup models are applied by first establishing the specific energy of the particle for the analyzed models. With this, an average value of S and t_{10} is calculated for several repeated cases for each rotor speed due to the randomness that exists in establishing the specific energies for the particles in DEM simulations [22]. The average value of t_{10} for each of the rotor RPM values obtained from the application of the breakage models to solid particles' speeds is contrasted with the average value obtained from five simulations with breakage for each of the rotor speeds.

For the application of the Tavares's model, the t_{10} variation for a single particle is taken into account:

$$t'_{10} = M\left(1 - \exp\left[-\frac{b' \cdot \kappa \cdot E_k}{E}\right]\right) \tag{14}$$

where E is the specific fracture energy of the particle and the variable κ is calculated by:

$$\kappa = \frac{\bar{E}_b}{E_{50b}} \tag{15}$$

In the last expression E_b is the mean fracture energy in the case of the upper log-normal distribution. The calculation of the variable κ is shown in [22]. The average results for both the simulations with breakage using the Rocky DEM [11] software and those obtained from the application of the breakage models to the particle speeds are shown in Fig. 8.

Figure 8 shows that both the results obtained from the simulations with breakage using Rocky DEM and those obtained from the application of the breakage models to the particle speeds present high randomness due to the way the specific fracture energy is set [22]. The increasing trend in the values of t_{10} is observed as the RPM of the rotor increases, except in some cases as in the 1500 RPM for the application of the breakage models and as in the 1300 RPM for the simulation with breakage, this trend is not maintained.

From the figure, it is observed that despite the randomness of the specific fracture energy leading to different results when an impact occurs, the application of both the Vogel & Peukert's model and the Tavares's model can represent the values of t_{10} that would be obtained if simulations including breakage were performed continuously.

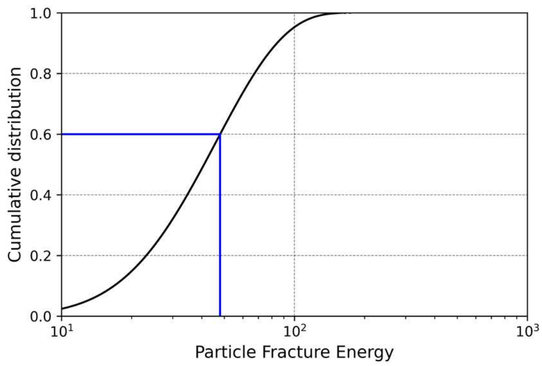

Fig. 7. Process for obtaining random specific fracture energy for particles in DEM simulations.

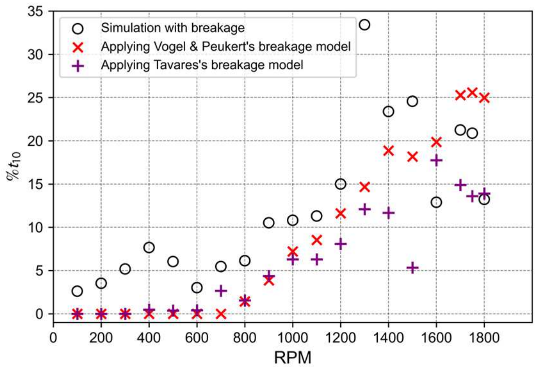

Fig. 8. Variation of t_{10} value as impact rotor RPM varies for single particle.

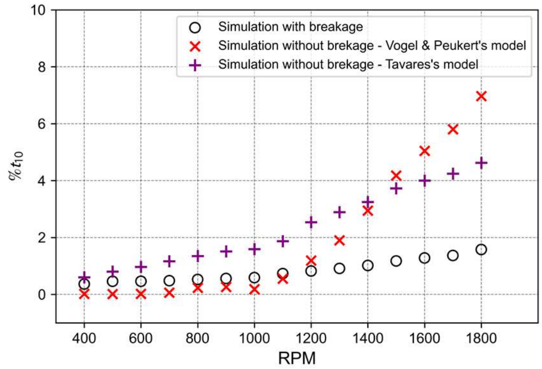

Fig. 9. Variation of t_{10} value as impact rotor RPM varies.

6.2. Particles Flow Impact into One Rotor with RPM Variation

In this second scenario, the first step for the application of the breakage models to particle speeds is to establish the specific fracture energy following the procedure mentioned above.

The average t_{10} values are calculated for both simulations with solid particles without breakage and for simulations applying continuous breakage. The average results of t_{10} values for both types of simulations are shown in Table 2 and Fig. 9.

The average value of five simulations for each speed is used because the simulations, regardless of whether they apply breakage or not, are not deterministic processes and therefore different values are obtained when the same simulation is performed again. Figure 9 shows that spites the variability obtained in the results of the DEM simulations, the increasing trend is maintained and the average values of t_{10} increase as the rotor speed increases. This happens because an increase in RPM leads to a higher value of impact energy and, therefore, a higher value of t_{10}.

In this same figure, it can be observed that Vogel & Peukert's model [9] produces higher t_{10} values than Tavares's model [10], especially for rotor speeds higher than 1200 RPM. This is because the t_{10} calculation, according to Vogel & Peukert's model, is the product between the t_{10} maximum value and the breakage probability. Although the latter, for a given energy, is lower than the breakage probability calculated by the Tavares's model, the Vogel & Peukert's t_{10} value is much higher because the factor used by Tavares's model that multiplies M in the t_{10} calculation (Eq. 10) is less than the value of S for the Vogel & Peukert's model.

As a result, for high energy impacts such as those from 1200 RPM or more, the t_{10} obtained by Vogel & Peukert's model is higher than the one obtained by Tavares's model. Figures 10 and 11 show the almost linear correlation that exists between the values of t_{10} obtained by applying the breakage models to the speeds and those obtained directly from simulations that include breakage. It can be observed that the results obtained from applying Tavares's model to the speeds of solid particles have a much higher R^2 correlation because the commercial software Rocky DEM also implements Tavares's model for breakage calculations.

Table 2. t_{10} results from simulations with continuous breakage and simulations with solid particles with the application of the models to particle speeds in simulations with varying rotor RPMs.

RPM variation			
RPM	Simulation with Breakage	Solid Simulations	
		Model [9]	Model [10]
400	0.364596	0.017967386	0.60385761
500	0.4611404	0.013301998	0.80145959
600	0.4619102	0.022792562	0.96987055
700	0.4821476	0.06492	1.16537226
800	0.5260306	0.230907151	1.35207341
900	0.560158	0.261641405	1.51132334
1000	0.5907558	0.180888571	1.59285057
1100	0.7318856	0.555908307	1.86937294
1200	0.8228026	1.192753391	2.53862564
1300	0.9132814	1.901762146	2.88879649
1400	1.0177934	2.947355951	3.2516577
1500	1.175922	4.177984189	3.72886574
1600	1.281142	5.045148164	4.00069006
1700	1.368122	5.80442031	4.24265714
1800	1.578036	6.973707361	4.62558633

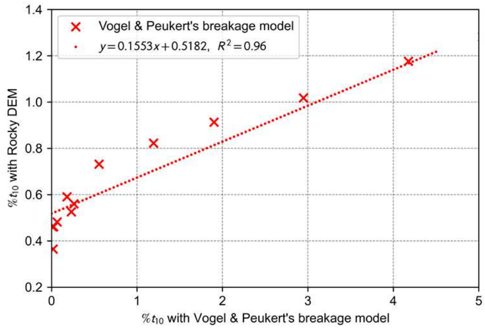

Fig. 10. Comparison of the estimated t_{10} values with those obtained with simulation with breakage for the model [9] when RPM is varied.

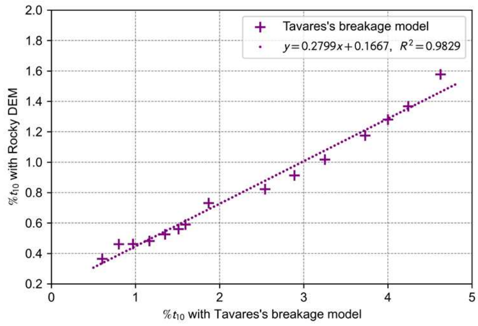

Fig. 11. Comparison of the estimated t_{10} values with those obtained with simulation with breakage for the model [10] when RPM is varied.

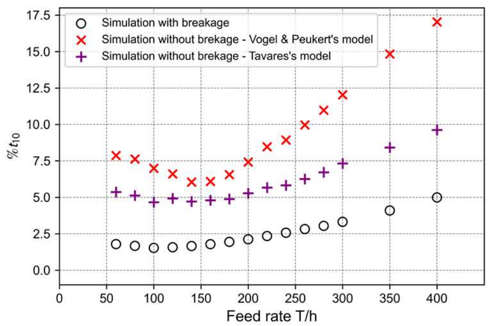

Fig. 12. Variation of t_{10} value as feed rate varies.

6.3. Particles Flow Impact into One Rotor with Feed Rate Variation

In this third scenario, after setting the specific energies randomly and applying the breakage models to the particle speeds, a trend similar to the previous case is observed. Higher t_{10} values are obtained as the feed flow increases; however, the increment seems to occur at a much higher rate at higher feeding rates. The results of the simulations corresponding to this second scenario are shown in Table 3 and Fig. 12. In this figure it is observed that both for the simulations with breakage and the application of the models [17, 18] in simulations with solid particles there is, at values lower than 120 T/h approximately, a slightly decreasing trend; however, from this minimum value, the trend increases.

Table 3. t_{10} results from simulations with continuous breakage and simulations with solid particles with the application of the models to particle speeds in simulations with feed rate variation.

Feed rate variation			
Feed rate	Simulation with Breakage	Solid Simulations	
		Model [9]	Model [10]
60	1.788184	7.870542116	5.3683189
80	1.668724	7.624885189	5.12729954
100	1.527692	6.989328783	4.6661265
120	1.571806	6.606173138	4.91994571
140	1.657726	6.043242146	4.7194136
160	1.78324	6.089317999	4.79411935
180	1.942926	6.557212901	4.88026074
200	2.119996	7.424949242	5.28587536
220	2.342902	8.468961683	5.67123898
240	2.568792	8.93427233	5.82849967
260	2.821674	9.96390827	6.25255275
280	3.040848	10.97419746	6.71782218
300	3.317248	12.03826504	7.32964458
350	4.094002	14.83255528	8.41218993
400	4.989442	17.03895431	9.62351628

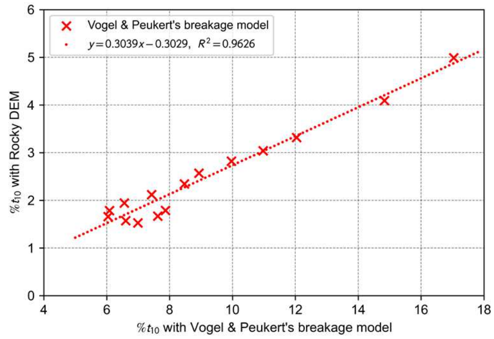

Fig. 13. Comparison of the estimated t_{10} values with those obtained with simulation with breakage for the model [9] when the flow rate is varied.

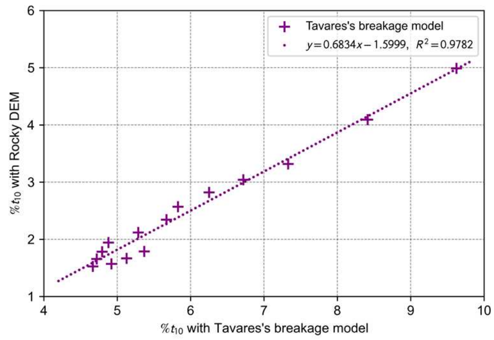

Fig. 14. Comparison of the estimated t_{10} values with those obtained with simulation with breakage for the model [10] when the flow rate is varied.

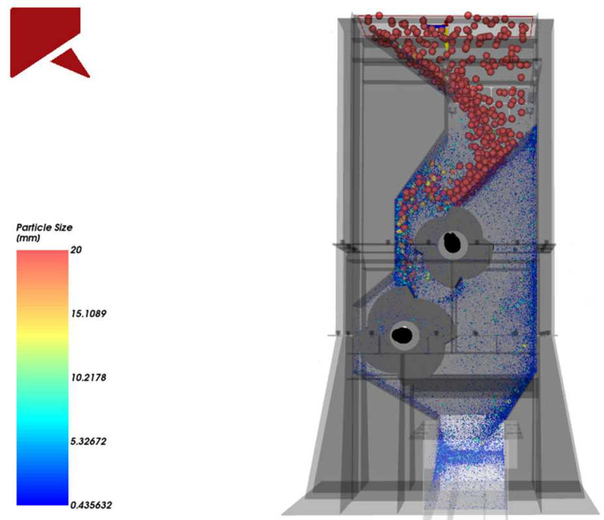

Fig. 15. Simulation with breakage of double rotor impact equipment.

Figures 13 and 14 show similar behavior to that observed in the RPM variation scenario. It is found that there is a linear correlation between the t_{10} results produced by the simulations with breakage and those obtained from the application of the models [17, 18] to the particle speeds. In the same way, as in the previous scenario, a higher value of R^2 is found when Tavares's model is applied to the particle speeds because the Rocky DEM software uses the same model for the breakage calculations.

6.4. Particles Flow Impact in Double Rotor Equipment with RPM Variation

To analyze the possibility of the application of the procedure shown in the present work in real equipment where breakage events are not always represented only by direct impacts between particles and rotors, the double rotor impact equipment is shown in Fig. 15 is presented. This equipment consists of two rotors of different sizes rotating at the same speed and positioned in such a way that the flow of broken particles produced by the upper rotor is directed and broken again by the lower rotor. This effect of both rotors causes the procedure shown in the present work to be not the most adequate as mentioned in the previous sections. The different results are because the speeds obtained in solid particle simulations contain impact speeds of particles against the lower rotor which do not exist in simulations that include breakage because these particles have already been broken in the upper rotor.

To determine the values of t_{10} obtained by applying the breakage models to the particle velocities for all rotor RPMs, the effects of the two rotors first are independently examined. Two different simulations are run for this purpose in the same manner as in the earlier sections. The first type consists of simulations that take into account the breakage for all chosen rotor RPMs. In these three scenarios, both the impact of both rotors operating simultaneously as well as the impact of one rotor operating independently while the other is left stationary are simulated. The second type of simulations omits breakage and repeats the previous process, yielding data for the combined impact of both rotors as well as for each one separately. Figures 16, 17, and 18 compare the outcomes of using the current technique for instances in which only one rotor and both rotors are operating.

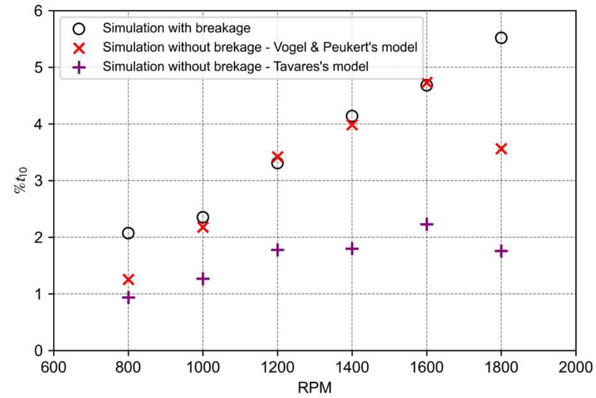

Fig. 16. Variation of t_{10} values obtained from both rotors as the RPM of both rotors varies.

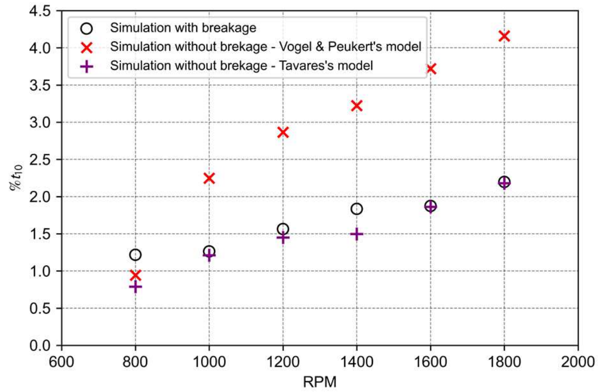

Fig. 17. Variation of t_{10} values obtained from the upper rotor as the RPM varies.

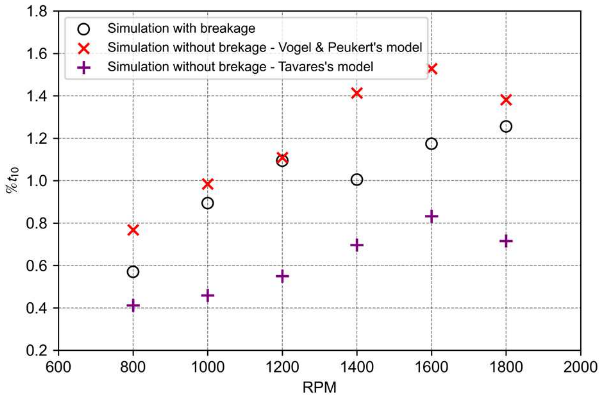

Fig. 18. Variation of t_{10} values obtained from the lower rotor as the RPM varies.

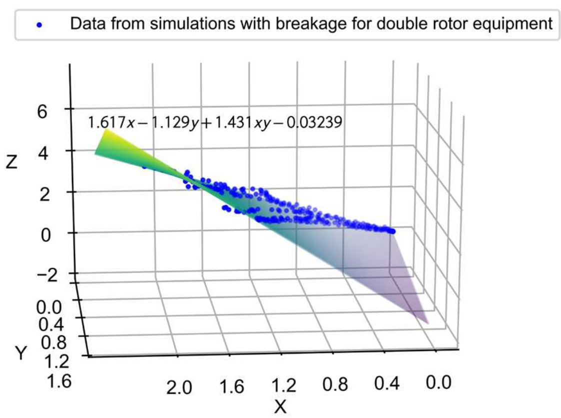

Fig. 19. Estimation of the effect of both rotors using the individual and combined effect of the upper and lower rotor. Equation of the form $ax+by+cxy+d$, $R^2 = 0.9738$.

From the above figures, it is observed that the application of the breakage models to the particles' speeds is adequate only in cases where one rotor is operating because the proposed procedure only takes into account the first breakage event. However, in order to estimate the effect of both rotors using the present procedure, it is established that the combined effect of both rotors can be equal to the effect of each rotor individually plus a combined effect produced by both rotors and an external effect. For the upper rotor the x value represents the value of t_{10} caused by it while the lower rotor is represented by y, $x.y$ is the effect of both rotors and d is an external effect, then the combined effect when using both rotors in operation, z is modeled by the following equation:

$$z = f(x,y) = ax + by + cxy + d \tag{16}$$

All t_{10} results obtained by using both rotors in operation (z) are adjusted by the results obtained from each of the rotors separately (x, y). The results are the product of the simulation with breakage of a particle flow double rotor equipment for various RPM values ranging from 800 RPM to 1800 RPM. The result of this fitting is shown in Fig. 19.

The fitting of the combined effect of both rotors by the individual effects was used to estimate the effect of the double rotor impact equipment using the particles' speeds for simulations with solid particles. The models were applied to the speeds obtained from each rotor individually and by fitting the individual effects to the effect of both rotors in operation, the t_{10} values produced by the complete equipment can be estimated. Figure 20 shows the linear trend obtained when comparing the results obtained by applying the breakage models and the z adjustment with the values obtained from simulations with breakage using Rocky DEM. It is observed that the application of Tavares's model obtains a higher R^2 value, and this is because the Rocky DEM software uses the same breakage model.

7. Discussion

Only the initial impact event for each particle is taken into account in the simulations with solid particles in the current work since subsequent events may not occur in simulations that do include breakage if the particle has already been broken and replaced by its progeny particles. For this reason, the results of applying the breakage models to the particle speeds at initial impact were compared to the t_{10} values obtained from the simulations with breakage.

The linear trend between the results obtained from simulations with solid particles and the results obtained from simulations with breakage for both RPM variation and feed flow variation is shown in Figs. 10, 11, 13 and 14. It is observed that the linear trend when using the Vogel & Peukert's model has a lower R^2 than when using the Tavares's model so that the latter can be used to predict the values of t_{10} for a solid particles' speeds. The high R^2 value is because the Rocky DEM software uses this model for breakage calculations. The results show a trend that allows the consideration that the t_{10} values resulting from simulations with breakage can be estimated by applying the models to the particles speeds of simulations with solid particles on equipment whose first impact is the most significant. This approach allows to reduce the simulation time considerably since, in the case of RPM variation, the simulations with breakage usually take about one hour while the application of the models to the speeds only takes five minutes on average.

A different case represents the analysis of the feed flow variation, since the number of particles increases considerably with more T/h, and so does the simulation time of models with breakage. For example, in the simulation of an inlet flow of 300 T/h more than fourteen hours were used compared to the five minutes it takes to simulate with solid particles and apply the model to the speeds. The difference between the results obtained from the breakage models applied to the solid particles' speeds and the results of the simulations with continuous breakage may be due to:

- Spurious impacts may appear in the particles' speeds since the particles that should break are kept in the simulation as solid particles. These fictitious impact events lead to higher values of t_{10} when the breakage models are applied to particles' speeds.
- The random specific fracture energy set for each particle in the simulations with breakage in Rocky DEM and in the application of the breakage models to the particles' speeds causes variability in the results produced.
- The breakage models applied to the solid particles' speeds only take into account the first impact and do not account for subsequent impacts of the particles, i.e., part of the energy produced due to the second and subsequent impacts is neglected. However, this neglected part of the energy is not reflected in the results since higher values of t_{10} are obtained when the breakage models are applied to the speeds compared to the values of t_{10} produced in the simulations with breakage by Rocky DEM. This contradictory result may be influenced by the spurious impacts mentioned above and by the algorithm used by the Rocky DEM for obtaining product particles since in the present work we have used those t_{10} values obtained after the generation of product particles, i.e., t_{10} values obtained in the post-processing stages of the DEM simulations.

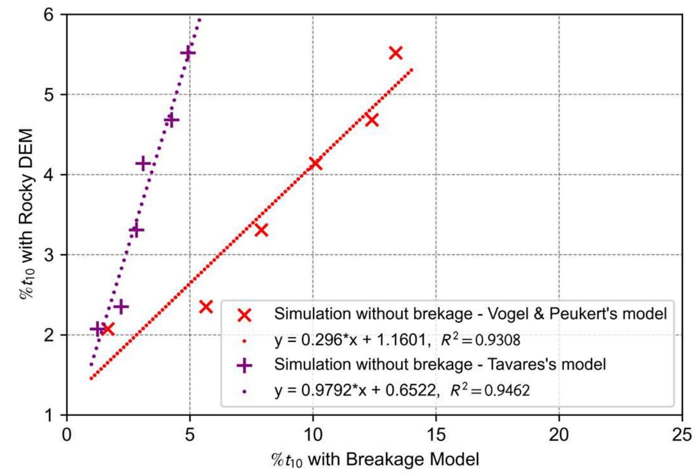

Fig. 20. Estimation of the t_{10} values produced by simulations with breakage in both rotors by applying breakage models to the individual kinematics of each rotor.

8. Conclusions

This paper identified a relationship between simulations with solid particles and simulations involving breakage. The speeds are processed using an algorithm that identifies the impacts through the variation between speeds and applies the breakage models [17, 18] for both single particle and a particle flow simulation. Parameters such as RPM and flow rate variation were studied. Finally, this method is used to estimate the value of t_{10} produced by a double rotor impactor.

The results showed that:

1. For both simulations varying the rotor RPM and those where the flow is varied, there is a linear relationship between the results obtained with breakage and those obtained using particles' speeds. A minimum value of R^2 of 0.96 and a maximum value of 0.9829 was obtained for the scenarios of RPM and feed rate variation for a particle flow.
2. Both models present variability in the results obtained for a single particle as opposed to what is obtained for a flow of particles where generally a more stable behavior is obtained; however, it is observed from the application of the Tavares's model that the variability in the results is due to the algorithm used to establish the specific fracture energy of the particles. In addition, it is observed that Vogel & Peukert's model, spite giving a higher resistance to the particles, models a more severe breakage than the one calculated by Tavares's model.
3. For equipment whose first impact is the most important, it is only necessary to calculate the first breakage event for each particle that breaks and with this result, it is possible to estimate the t_{10} values obtained when the breakage is calculated continuously in simulations that include breakage.
4. The similarity in the behavior of the t_{10} values allows us to think that, for equipment whose first impact is the most important, the results of complete simulations that include breakage can be estimated using the procedure presented in this article. However, other studies involving different materials and the variation of more particle parameters, as well as the use of other impact rotors, such as those used by vertical and horizontal shaft impactors (VSI and HSI), still need to be carried out.

Author Contributions

M.A. Castro planned the scheme, conducted the experiments, examined the theory validation, analyzed the empirical results, and write the original draft; J. Yarasca developed the methodology, suggested the experiments, formal analysis, and review and editing the original draft; A.J. Castro conducted the data curation, formal analysis, and development of the software; J.L. Mantari planned the scheme, initiated the project, suggested the experiments, formal analysis, project supervision and review the original draft. The manuscript was written through the contribution of all authors. All authors discussed the results, reviewed, and approved the final version of the manuscript.

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Conflict of Interest

The authors declared no potential conflicts of interest concerning the research, authorship, and publication of this article.

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Data Availability Statements

The datasets generated and/or analyzed during the current study are available from the corresponding author on reasonable request.

Nomenclature

b'	Material parameter includes the effect of particle size	S	Probability of breakage [%]
f_{MAT}	Material parameter [kg.J^{-1}m^{-1}]	t_{10}	Breakage severity [%]
M	Maximum t_{10} value	x	Particle size [mm]
$P(E_k)$	Probability of particle breaks [%]	γ	Damage accumulation parameter

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