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VALIDATION OF BREAKAGE MODEL IN THE DISCRETE ELEMENT METHOD BY SIMULATION OF SINGLE PARTICLE IMPACT

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Abstract. *The discrete element method (DEM) is a powerful tool to describe the behavior of particulate flows, however when simulating particle handling in DEM environments, breakage is not considered in most of the cases due to the limitations presented by different techniques available currently. When simulating particles that are subjected to breakage, its absence may lead to erroneous results and this situation becomes critical when simulating systems that are meant to perform particle breakage during operation, as crushers and mills used across different areas of study. The work uses the new model implemented in the commercial DEM platform Rocky DEM 4.1 (Tavares Breakage Model) to replicate bench-scale tests used in mineral industry for ore characterization. The work demonstrated that the model has potential to describe particle breakage, comparing numerical results from the model with results achieved in simulation.*

Keywords: *Discrete element method, particle breakage, comminution, Rocky DEM*

1. INTRODUCTION

The discrete element method (DEM) is a numerical method that allows simulating motion of a large number of particles in a granular medium through the application of Newton's second law of motion and contact models (Jiménez-Herrera *et al.*, 2017) to predict the interaction between particles and particles and their environment. The use of software to simulate DEM allows the estimation of important information during and after its processing, such as flow rates, collisional and work distributions, dynamic loads on boundaries, wear rate and so on (Cleary, 1998), constituting a powerful tool to evaluate engineering problems in granular materials.

Particle size reduction is a key process in a wide range of applications across different areas. In the minerals industry it is used in the production of fine and coarse aggregates (aggregate industry), in liberation of valuable minerals from gangue (mineral processing) and in preparation of raw materials and clinker (cement industry) (Weerasekara *et al.*, 2013). Extensive research has been done in recent years to understand the breakage phenomena, improving and optimizing rock crushing processes. The adoption of the discrete element method is a potentially important step to understand the behavior of particulate flow on crushers and mills, reducing their inefficiency and allowing the readily evaluation of the equipment design and operational conditions (Quist & Evertsson, 2010).

The absence of a description of breakage when simulating flow of particles in several applications using DEM may lead to biased results. On the other hand, this absence is critical when simulating systems that are meant to perform particle breakage during operation and the bulk flow of material is strongly dependent on a proper description of particles breakage. Examples of these are gyratory, cone crushers and high pressure grinding rollers. In simulating these equipment using DEM, different approaches have been used recently, which include the bonded-particle model (BPM), in which a set of spherical particles are bonded together in each contact point using bonding beams (Potyondy & Cundall, 2004), and the particle replacement model (PRM), in which a set of progeny particles replaces each particle after a breakage event (Cleary, 2001). A few examples adopting these models can be found in Quist *et al.* (2011), Johansson *et al.* (2016), Delaney *et al.* (2015) and Barrios & Tavares (2016). Although these approaches are able to describe with some success the fragment distribution of the progeny particles, they present some limitations, such as the lack of mass conservation whenever breakage occurs for both models, the elevated computational effort necessary to simulate breakage using BPM and the lack of breakage probability prediction using the PRM (Jiménez-Herrera *et al.*, 2017).

Single impact tests, such as the drop test, are widely used in ore characterization due to their ability to replicate the mechanism used in several comminution equipment, such as mills and impact crushers. Using the new Tavares Breakage Model implemented in the commercial DEM platform Rocky DEM 4.1, the present work aims to validate DEM simulation results with numerical results of the model previously calibrated for a variety of materials (Tavares, 2004, 2009; de Carvalho & Tavares, 2013).

2. MODEL DESCRIPTION

The named Tavares Breakage Model, implemented in Rocky DEM 4.1, comprises a series of equations proposed by Tavares (2004, 2009) to model the phenomena of particle breakage. The model accounts for rock properties that are not fully covered by other breakage models already in use in DEM environment. Besides the fact that the model as implemented in Rocky DEM is capable of conserving mass and volume and generating non-rounded polyhedral fragments after a breakage event, it also accounts for the variability in strengths of particles, even for the ones with the same size and material composition. According to the model, the distribution of particles fracture energies of a particular size fraction of the material can be readily estimated from the breakage probability distribution $P_o(E)$, that is represented by the upper-truncated lognormal distribution (Tavares, 2009), given by

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

where

$$E^* = \frac{E_{max}\, E}{E_{max} - E} \tag{2}$$

where E_{max} is the upper truncation value of the distribution, E_{50} is the median particle fracture energy and σ^2 is the variance.

The model also accounts for the increase in the mean strength of particles as they become finer (de Carvalho & Tavares, 2013). This dependence is calculated based on the size of interest, according to equation

$$E_{50} = E_\infty \left[1 + \left(\frac{d_o}{L}\right)^{\varphi}\right] \tag{3}$$

where E_∞, d_o and ϕ are model parameters fitted to experimental data and L is the representative size of the size class of interest.

When the energy involved in a collision is lower than the fracture energy of the particle, it will not lead to breakage. However, the particle may become more amenable to break on a subsequent stressing event due to the accrual of internal damage (Tavares & King, 2002). The particle weakening is described on the basis of elements from continuum damage mechanics and the damage sustained in the *n*th cycle is given by

$$D_n^* = \left[\frac{2\gamma}{(2\gamma - 5D_n^* + 5)} \frac{E_{k,n}}{E_{n-1}}\right]^{\frac{2\gamma}{5}} \tag{4}$$

where γ is the damage accumulation coefficient, $E_{k,n}$, the contact specific energy and E_{n-1} is the particle energy threshold. Every time $E_{k,n}$ is greater than the E_{n-1}, breakage will occur. If not, the particle will accumulate the damage and the energy distribution will be given by

$$E_n = E_{n-1}(1 - D_n^*). \tag{5}$$

Whenever breakage occurs, the size of the progeny particles will mainly be governed by the parameter t_{10}, which corresponds to the percent in weight of the original particle that passes through a sieve with aperture equal to 1/10th of its original size ((Tavares, 2009). This extent of breakage is related to both stressing conditions and material fracture energy according to equation

$$t_{10} = A\left[1 - \exp\left(-\frac{b' E_{k,n}}{E_{50b}}\right)\right] \tag{6}$$

where A and b’ are model parameters fitted to experimental data and E_{50b} is the median particle fracture energy of the particles that were broken in the particular stressing event.

Whenever particles are subject to impacts that are not capable of breaking all the particles in the first impact, E_{50b} will no longer be the same as E_{50} and the median fracture energy of particles that break in the first impact must be calculated according to equation

$$E_{50b} = E_{50}\, exp\left[\sqrt{2}\sigma erf^{-1}(P_o(E_k) - 1)\right]. \tag{7}$$

The full-size distribution of particles is estimated by Rocky DEM 4.1 based on either the Gaudin-Schuhmann distribution or the incomplete beta function distribution, given by, respectively

$$\%Passing = \frac{t_{10}\,.x}{0.1L} \tag{8}$$

$$t_n(t_{10}) = \frac{100}{\int_0^1 x^{\alpha_n - 1}(1-x)^{\beta_n - 1}dx} \int_0^{t_{10}/100} x^{\alpha_n - 1}(1-x)^{\beta_n - 1}dx \quad (9)$$

where the cumulative mass of the particles passing a screen with size x is defined by the calculated t_{10} value and the original particle size L. The progeny particles are generated in DEM environment using the Voronoi subdivision algorithm (Potapov & Campbell, 1994).

3. SIMULATION SETUP

The commercial software Rocky DEM by ESSS has been used for DEM simulation. A set of 48 drop tests was designed for the purpose of this work, as presented in Fig. 1. Particles of 5.47 mm in size, comprising the size range of 4.75 to 6.30 mm, of copper ore and limestone were used in the simulations. The choice for these materials was due to the difference between their breakage strengths. The particles were generated on a inlet situated one meter above the anvil with a initial normal velocity to simulate greater heights. Figure 2 shows the shape adopted for both materials in order to mimic the original shape of the particles.

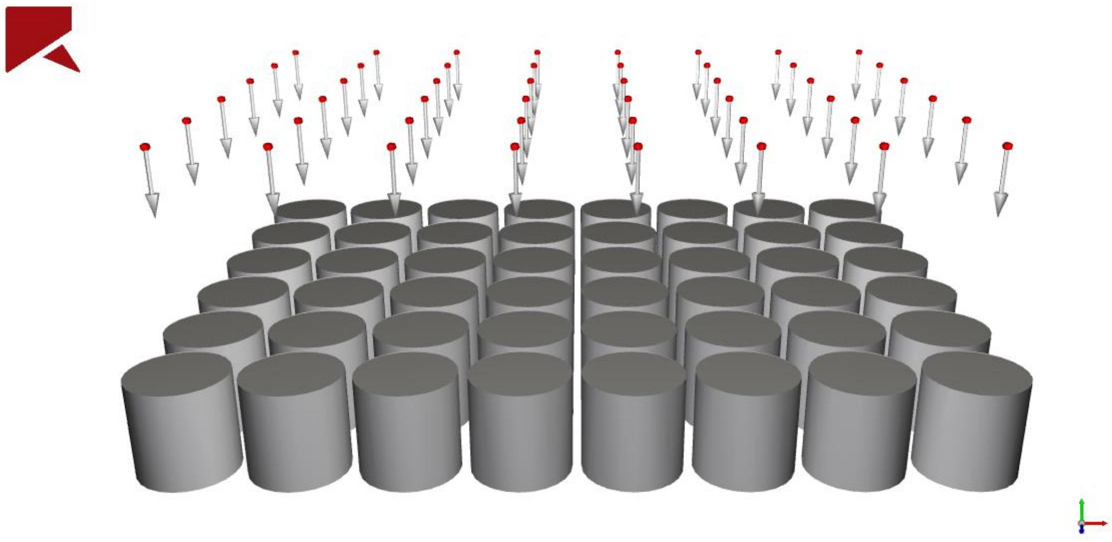


Figure 1 - Simulation setup of 48 single particle impact tests in DEM environment using particles of 5.47 mm.

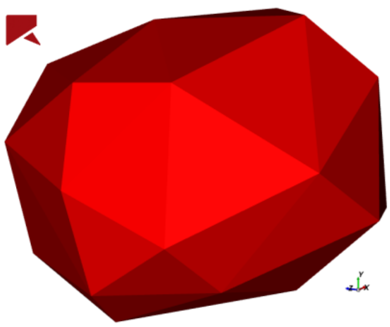


Figure 2 – Generic particle shape of a 5.47 mm particle adopted in the simulations.

The Tavares Breakage Model requires a set of parameters that can be fitted to experimental data using bench-scale tests. The procedures used to fit the model can be found elsewhere (Tavares, 2004, 2009). Table 1 presents the parameters used in all simulations, which may be found in different publications from the authors´ laboratory (de Carvalho & Tavares, 2013, Jiménez-Herrera e*t al.*, 2017). In order to reduce the computational effort, the minimum size of fragment produced by breakage was set as 0.25 mm.

Table 1 – Input parameters of the Tavares Breakage Model used in the simulations.

	Copper ore	Limestone
γ	5	5.4
σ^2	0.638	0.642
A	67.71	53.3
$b´$	0.0294	0.033
E_∞ (J/kg)	213.5	7
d_o (mm)	8.073	100
φ	1.219	0.8
E_{max}/E_{50}	4	4
$\alpha_{1.2}/\beta_{1.2}$	0.51/11.95	0.19/7.78
$\alpha_{1.5}/\beta_{1.5}$	1.07/13.87	0.56/7.51
α_2/β_2	1.01/8.09	0.78/5.55
α_4/β_4	1.08/3.03	1.12/3.01
α_{25}/β_{25}	1.01/0.53	1.17/0.54
α_{50}/β_{50}	1.03/0.36	1.43/0.40
α_{7}/β_{75}	1.03/0.30	1.92/0.42
Density (kg/m³)	2930	2710
Young's Modulus (N/m²)	5.22E+10	3.50E+10

4. RESULTS AND DISCUSSION

The simulation was carried out 16 times for each material, one for each impact energy, varying the breakage probability from 0.1% to 100%. In order to compare the accuracy of the model, the breakage probability and the t_{10} predictions for each scenario simulated was compared with the expected results from the numerical calculation, which has been previously fitted to experimental data. Additionally, the particle size distributions were collected right after the impact between the particle and the anvil and compared to the predicted distribution from the model using the incomplete beta function.

It is known that particles in a certain size range do not have the same fracture energy (Tavares & King, 1998). In Fig. 3 it is possible to observe that both the copper ore and the limestone particles presents wide spectra of fracture energies. The model was able to predict with accuracy the behavior of the particles fracture energies.

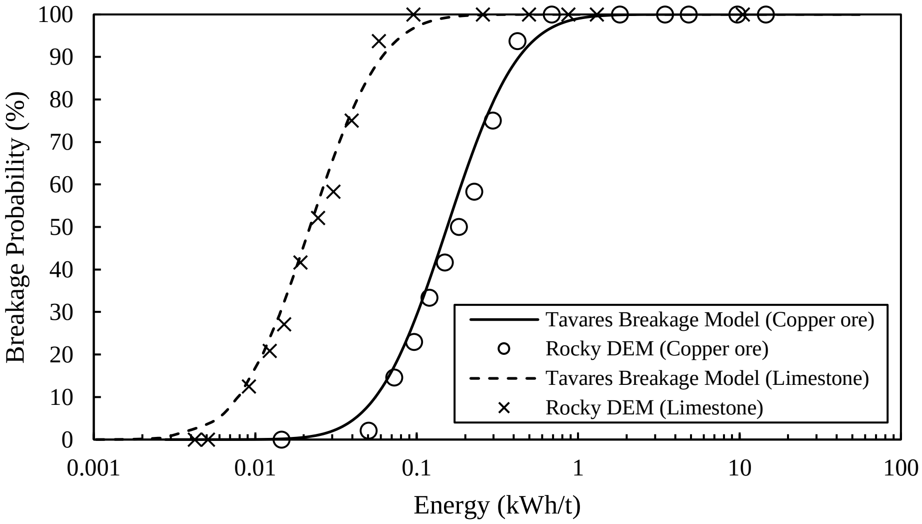


Figure 3 - Comparison between the modelled and simulated breakage probability for a single particle impact of particles of 5.47 mm for different impact energies.

Yet, another important parameter to verify the accuracy of the model is the fineness of the breakage product. Figure 4 presents the expected t_{10} values of the model and the values observed in simulations. The parameter *A* of the model, as shown in Eq. (6), can be interpreted as the maximum expected value of $t_{10,}$ indicating that the particle breakage reaches a saturation level and higher energies will not lead to finer distributions of the product. The simulations presented good adherence for the modeled t_{10} values for higher energies but underpredicted values for lower energies.

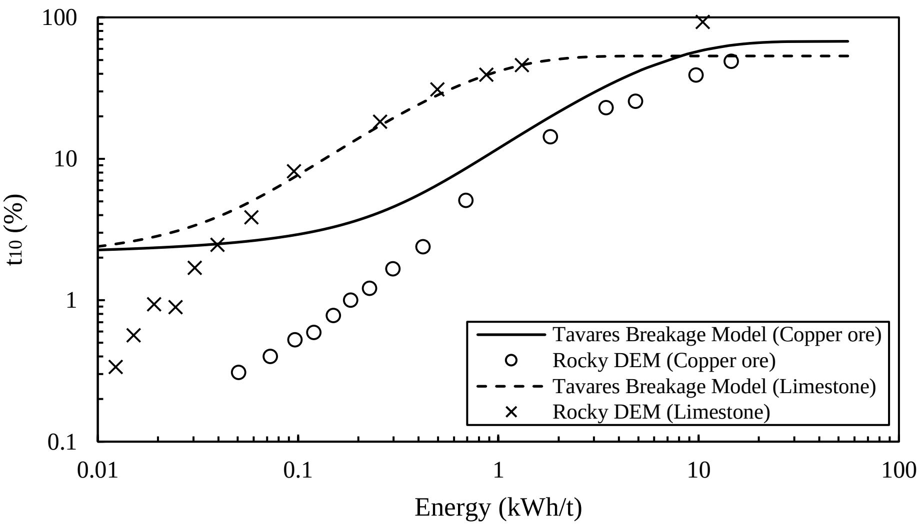
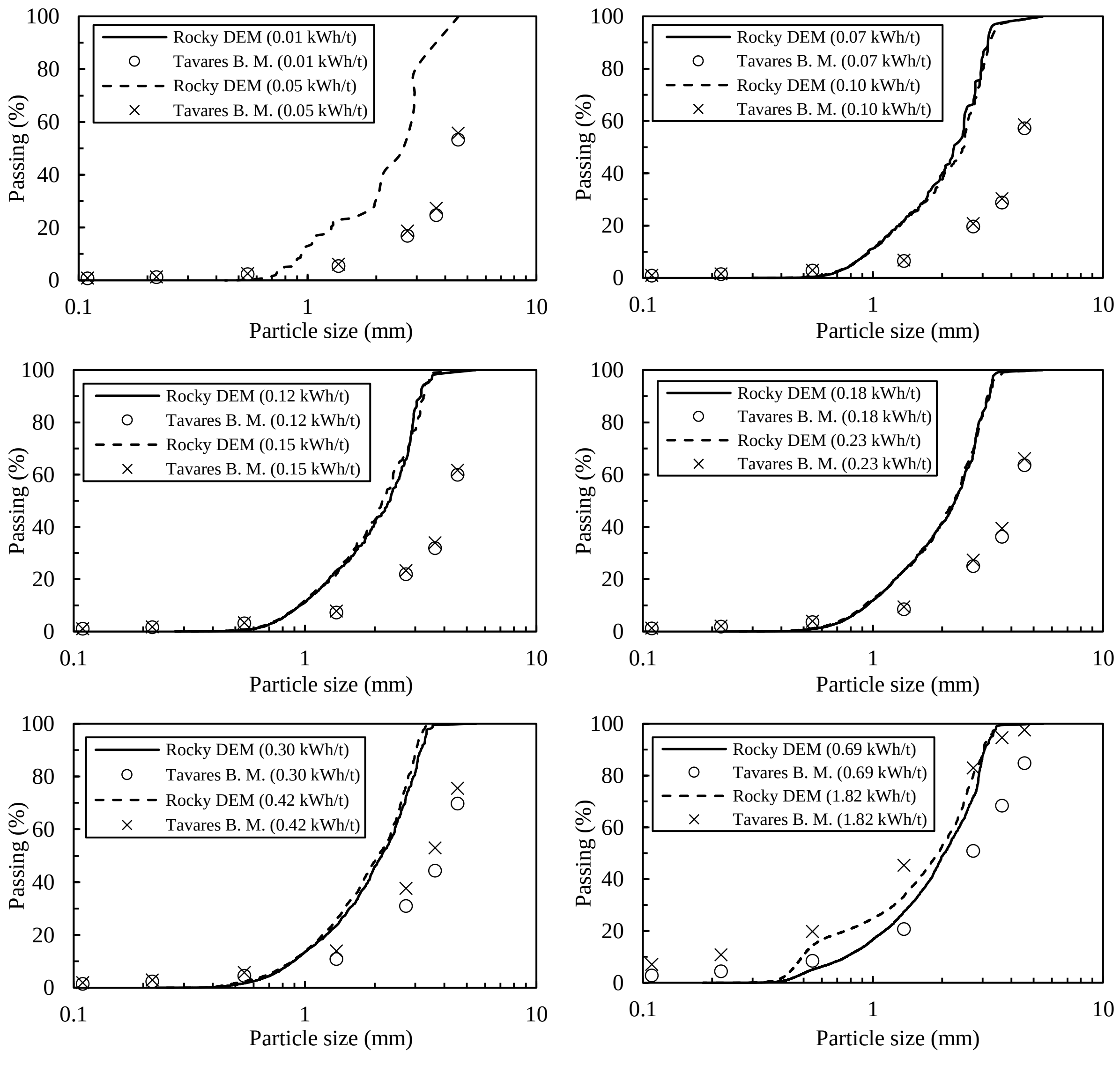


Figure 4 - Comparison between the modelled and simulated t_{10} values for a single particle impact of particles of 5.47 mm for different impact energies.

In Fig. 5 and Fig. 6, the simulated particle size distributions are compared to the numerical results using the incomplete beta function for the copper ore and the limestone particles, respectively. The simulation reproduced correctly the expected behavior, generating finer fragments when submitting the original particles to an impact at a higher collision energy. For both materials, the simulation presented better adherence for medium impact energies, whilst overestimating the breakage for low impact energies and underestimating it for higher energies. As mentioned, the minimum fragment size of 0.25 mm was selected, so that no particles below this size appear in the simulation results.



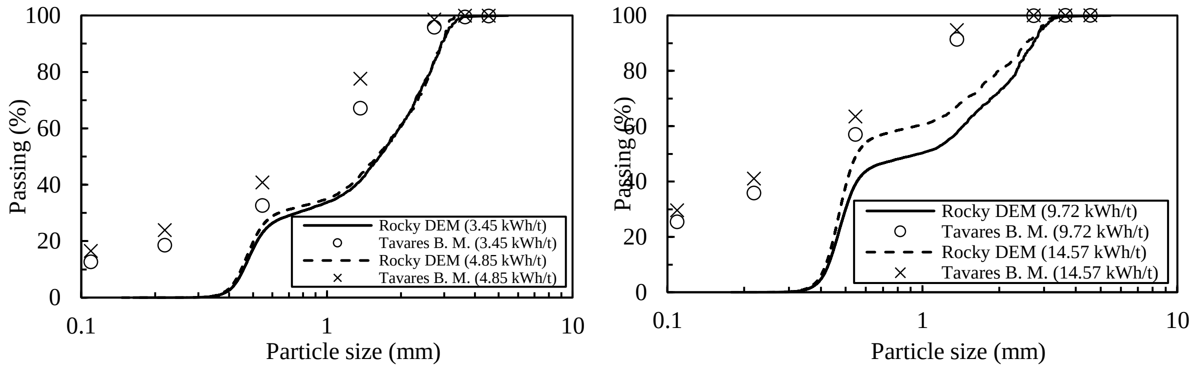
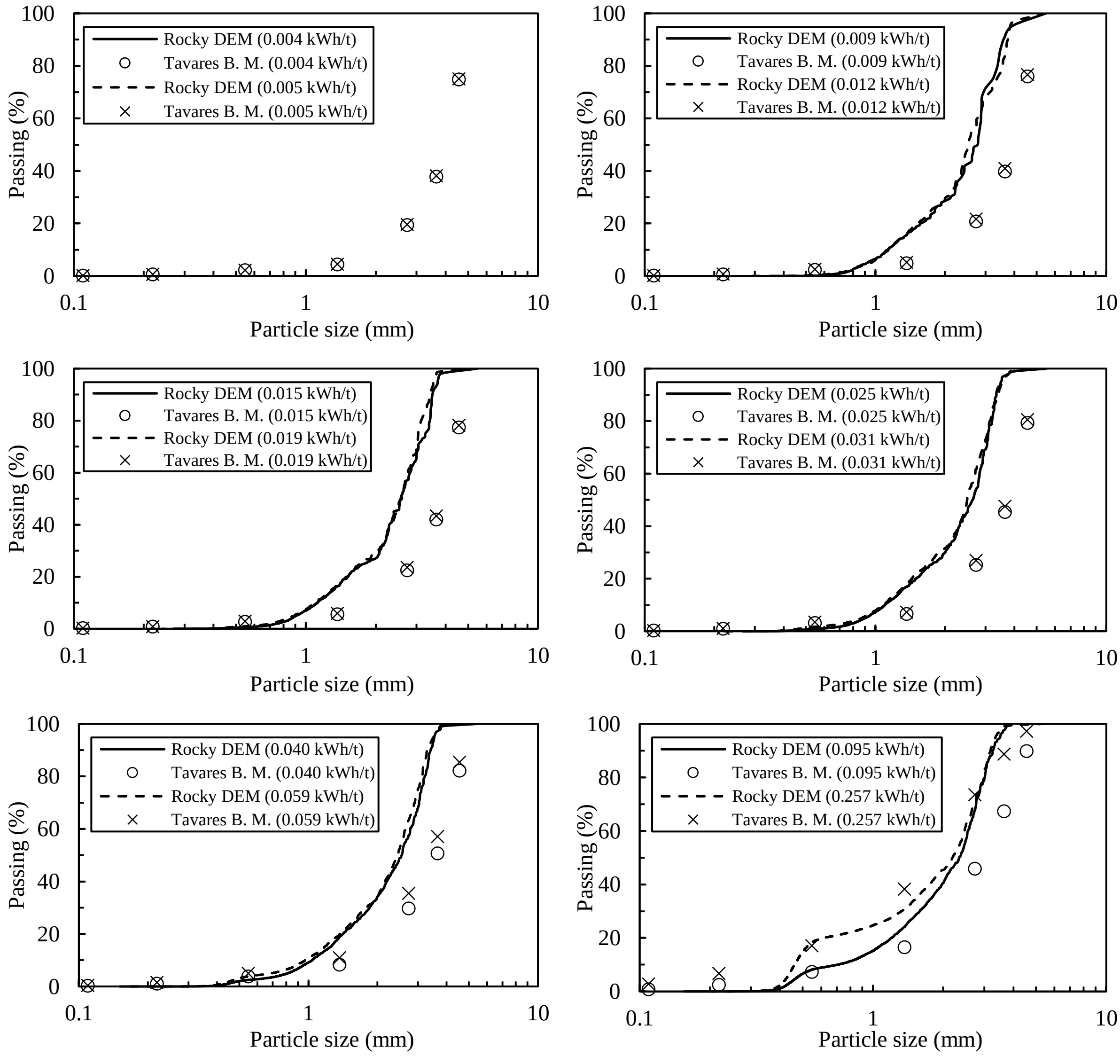


Figure 5 – Comparison between the modelled and simulated progeny size distributions for a single particle impact of particles of 5.47 mm for different impact energies for the copper ore particles.



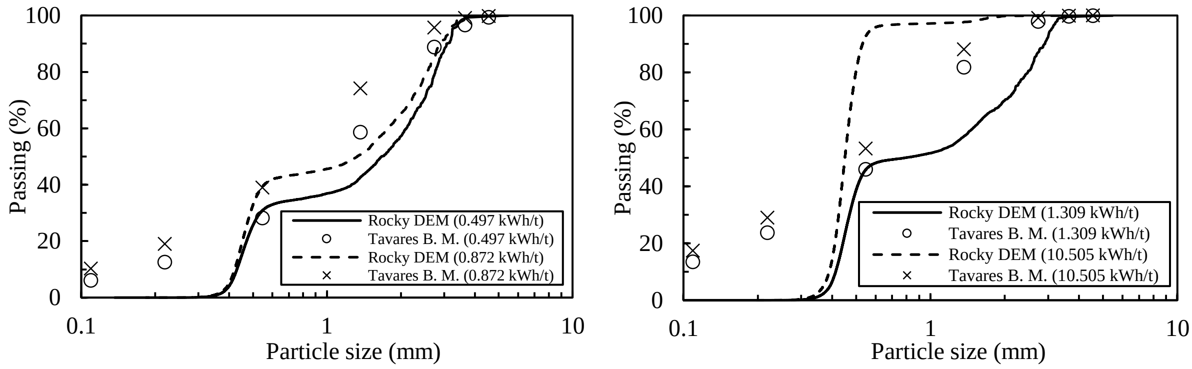


Figure 6 – Comparison between the modelled and simulated progeny size distributions for a single particle impact of particles of 5.47 mm for different impact energies for the limestone particles.

5. CONCLUSIONS

The Tavares Breakage Model available in the commercial DEM platform Rocky DEM 4.1 has been tested for single impacts on particles of materials of different strengths to validate the software predictions. The model as implemented presents benefits over traditional techniques already in use to emulate breakage in DEM environment, especially due to the mass and volume conservation after a breakage event, its fidelity describing several aspects of particle breakage and its simplicity in parameter fitting.

The model predicted the progeny size distribution from single-particle drop testing with reasonable accuracy, specially when comparing values of t_{10} at high-energy impacts. The model was also accurate in the prediction of the breakage probability curve.

Single particle impacts are a good way to validate breakage models due to the simplicity of the breakage mechanism. Although in the early beginning of its development, the model presented good results and can easily replace other breakage methods adopted in DEM environment. More work is, however, needed to validate the model using different bench-scale tests and large-scale comminution systems.

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