Experimental calibration methodology for numerical parameters in a DEM software based in granular material static tests

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Abstract. Simulations are one of the most used tools in different investigations and topics, being a powerful tool to replicate a real-life system or to solve real engineering problems without interrupting any process. To accomplish a reliable replication of the real system, it is necessary to make good assumptions in the numerical parameters selection of the simulation and its configuration. The main goal of this research is to propose a calibration methodology of numerical parameters based on static tests simulations in the Rocky-DEM software. A laboratory flow test experiment was developed to measure the repose (ar) and emptying (ae) angles of a granular material in a static state. In the simulation experiment, these angles are dependent of numerical parameters, such as the static friction coefficient (mf), the rolling coefficient (mr) and the adhesive distance (da). To get the best numerical parameters that explained the behavior in the laboratory experiment, an optimization procedure was done. Two materials were used for this research: chickpeas, for the development of the calibration methodology, and sulfide copper ore, to apply this methodology. The numerical parameters for the chickpeas experiment were mf = 0.183, mr = 0.105 and da = 0.938 [mm], resulting in ar = 31.23° and ae = 28.85°. These simulated angles have a variation of 2.85% and 3.03% with respect to the values obtained in the laboratory experiment. In the case of the mineral experimentation, a mf = 0.892 and mr = 0.269 were obtained, simulating a ar = 30.1° and ae = 42.31°. Also, these results have a variation of 2.84% and 3.65% with respect to the values of the angles measured in the laboratory model. As a conclusion of the study, DEM simulation is a powerful tool to predict the behavior of granular materials. However, it is necessary to use calibrated values and settings in the simulations to increase the accuracy of the results.

1. Introduction
The discrete element method (DEM) consists of representing the material discontinuously by a set of discrete particles. The discontinuities are considered as boundary conditions. The contact forces and displacement of the set of particles under a stress distribution are determined through a series of calculations involving their motion.

The DEM simulations are governed by mathematical equations that describe the behavior of the model and therefore its results. Every equation has numerical parameters that control the magnitude of these results [1], which is why these parameters are important to know and calibrate. Also depending on
the experiment type that is being replicated with simulations, it will be very important to know which and how many parameters will have a greater effect in the behavior of the model.

The main goal of this research is to develop a calibration methodology to estimate the numerical parameters in a DEM simulation. This methodology was applied in the estimation of the repose and drawdown angles in bulk material performed in a granular flow test [2]. This research is focused for DEM simulations because it is the best method for replicating a bulk material [3]. In this research we use the Rocky-DEM software.

In DEM simulations, the same procedure of the laboratory experiment is replicated. At the end of each simulation the repose and drawdown angles are measured. Finally, these results are compared with those obtained in the granular flow test.

2. Experimental set-up
The experiment chosen was a granular flow test, whose procedure and its respective set-up allowed to estimate the repose and drawdown angles. The repose angle [4] is commonly used to be measured in bulk material, while the drawdown angle measures the resulting slope when discharging gravitationally through the center of the base of bulk material [5] (Figure 1).

![Figure 1. (a) Repose and (b) drawdown angles](image)

The bulk material chosen was chickpeas due to its shapes, similar to spheres, allowing us to reduce the computational cost in the DEM simulations [6].

Both in the experimental test and DEM simulation, constant environmental values of temperature and humidity were used. Chickpea density is indirectly calculated by volume displaced in a test tube, resulting in a value equal to 1333 kg/m³, while for sulfide copper ore a value equal to 2600 kg/m³ with the same measurement method. The average size of chickpea grains was 8.5 millimeters in diameter with 15 kilograms of material used, while for the ore, it has a size distribution (table 1) with a maximum size of 19.1 mm and a total mass of 17.5 kg.

| Size (mm) | Cumulative (%) |
|----------|----------------|
| 19.1     | 100            |
| 12.5     | 90.05          |
| 9.5      | 87.3           |
| 6.35     | 0.1            |

Table 1. Size distribution for sulfide copper ore experiment and DEM simulation.

Using factorial design [7], the number of measurements is determined with respect to the number of parameters involved in the experiment (equation 1). In this case were: static friction coefficient, rolling resistance and adhesive distance. For each parameter, a lower and a higher level of possible values are
considered. For static friction coefficient the values are between 0.1 and 0.7, between 0.1 and 1.0 mm for adhesive distance, and between 0.1 and 0.5 for rolling resistance. As a result of the above, it is necessary to develop 8 experiments and simulations.

\[ \text{Numbers of Experiments} = \text{Parameter Levels}^{\text{Parameter Numbers}} \]  

For those parameters, whose values are not modified in the model, there is the following setting:

- Particle – Particle interaction: Both static and dynamic friction coefficients have a value equal to 0.5, 0.3 value for coefficient of restitution, 6.25 millimeters for adhesive distance, and a force fraction of 0.4.
- Particle – Boundary interaction: Static and dynamic friction coefficient have a value equal to 0.7, a coefficient of restitution of 0.3, an adhesive distance of 6.25 millimeters, and a force fraction of 0.4.
- Rolling resistance equal to 0.28.

Finished the preparations of experiments in laboratory and numerical model, it starts the experimental procedure of the granular flow test. The experimental mounting and the experimental procedure are detailed in Figure 2.

![Figure 2](image_url)

**Figure 2.** Design of the granular flow test mounting experiment (a) frontal view, (b) lateral view, (c) isometric projection and (d) experimental procedure diagram

The procedure to perform the granular flow test is as follows:

1. **Material treatment:** For maintain the same assumptions of bulk material such as distribution and particle shape, is done a treatment of material before of each measurement. Treatment as weight, screening and homogenization.
2. **Deposite in assembly:** Treated bulk material is deposited on upper part of the mounting, entering to the first chamber.
3. **Opening in upper chamber:** With material at rest, separation of boards is continued at a distance established by the experimenter (20 centimeters for this research). These tables boards correspond to the base of the first chamber. This allows the material to pass into the second chamber.
4. **Data collection:** Once the material comes to rest again, photographs are taken to the upper chamber, and to the lower chamber, where the drawdown and repose angle will be located, respectively. The photographs are taken with corresponding measurements of distance and height of the photographic camera, to reduce as much as possible the influence of perspective
in the angle photographs. To facilitate the image treatment task that will take place later, a green sheet is placed on the chamber background.

5. **Measurement and registration:** Photographs are processed by MATLAB software to measure the angles.

6. **Material removal:** Finally, the experiment is completed by removing the bulk material from the chambers. Then, it is return to point 1.

The experimental procedure must be reproduced into the numerical model, making a copy as exact as possible of the real experiment, changing only in each simulation the values of the numerical parameters of interest.

3. **Calibration methodology**

The diagrams of the stages of the resulting calibration methodology are shown in Figure 3 and Figure 4.

The first third of the methodology corresponds to the preparation of experimentation in the laboratory and DEM simulations, the choice of bulk material to be calibrated, the corresponding numerical parameters, the response variables and how and where they will be measured. The necessary considerations and simplifications for the simulations are also decided in order to avoid a higher computational processing cost, without compromising the calibration approach and its results.

**Figure 3.** Diagram of the first stage: preparation of base of the experiments
Figure 4. Second stage: development of laboratory experiment and DEM simulations

The intermediate stage corresponds to the experiment execution, simultaneously carrying out the laboratory procedure and the DEM simulations. Preliminary testing is recommended to observe aspects that may not have been considered in the preparation stage.

With the DEM simulations results, a response surface [8] of all possible values of angles is generated regard to numerical parameters that were varying in each simulation (static friction coefficient, rolling resistance and adhesive distance). Ansys DesignXplorer is used through the constant kriging interpolation type to create this surface [9].

An optimization to the response surfaces is carried out, using the MOGA type interpolation algorithm [10], to find the numerical parameters which assure to replicate the values obtained from the angle measurement of chickpeas and the ore in the experimental procedure.

For a higher accuracy in the calibration, it is used as a criterion the difference margin. This margin is associated to the standard deviation of the experimental measurement. Any optimization result that generates a response variable in DEM simulations outside the difference margin, is added to the data set to create a new response surface and be optimized again.

4. Results

4.1. Angle measurement

4.1.1. Experimental model. The experimental angle measurement is done by taking photographs to the repose and drawdown angles of the bulk material. The angle was determined by adding a green sheet to the chamber background and the bulk material. Then the photograph is converted into a binary image [6], that is, in an image with a white area that represent the material and a black area that correspond to the background. Subsequently, binary image is cropped, leaving the right and left side, discarding the upper part due to the sudden change in angle (Figure 5).
A set of points are generated at the intersection of both areas (black and white), in which it is possible to apply a linear regression to obtain the slope and subsequently determine the angle (Figure 6).

With angles obtained, the average angles of left and right sides are calculated and recorded, having an average repose and drawdown angle per measurement.

4.1.2. Numerical model. Angle measurement procedure in DEM model consists of performing a post-processing at the end of each simulation. Eulerian statistics are used, a tool present in RockyDEM [11], which allows the chamber volume to be discretized at the width and depth of the chamber, being divided several times with respect to the maximum particle size.

The tool makes it possible to request the particle centroid that reaches the highest position with respect to the height for each division made across the width for a division with respect to the depth of the volume chamber. By taking these points to a plot, the pile silhouette of bulk material is described and where it is possible to determine the left and right angles of this (Figure 7).

This process is repeated for each division regard to the chamber volume depth, from the chamber front to the rear, where left and right side are recorded in each one. Final calculation corresponds to average of previous data for each side and the side with a lower standard deviation is kept as the final result.

4.2. Chickpeas experiment
According to the experimentation and process carried out in laboratory to measure response variables for this bulk material, it was 30.36° ± 1.32° of repose angle and 28.00° ± 2.28° of drawdown angle.

From simulations, there are 8 design points where for values of the minimum levels for the numerical parameters that are 0.1 for static friction coefficient, 0.1 millimeters for adhesive distance and 0.1 for rolling resistance, is reached 29.45°±0.7° in repose angle and 27.89°±1.17° in drawdown angle. While for maximum values of 0.7 of static friction, 1 millimeter for adhesive distance and 0.5 for rolling resistance, is reached 33.88°±1.50° in repose angle and 47.78°±2.01°.
With the design points, the response surface and corresponding optimization are generated, reaching a calibration for chickpeas bulk material with values of numerical parameters 0.18 of static friction coefficient, 0.94 millimeters of adhesive distance and 0.105 of rolling resistance, resulting in DEM simulations response variable of 31.23°±1.34° for repose angle and 28.85°±0.77° for drawdown angle.

4.3. Sulfide copper ore experiment
Due to the complexity of its particle shape and the effect in the computational processing time, it was decided to simulate spheres. In this case, the numerical parameter of the adhesive distance is discarded, since this parameter tries to represent the cohesion/adhesiveness of bulk materials generally in the presence of water, however the ore material was treated with a low moisture content [5].

![Figure 7. Plot with simulation results, on the left the points that describe the repose and drawdown angle, and on the right side the angle magnitude with respect to the chamber volume depth](image)

Average angle for copper sulfide ore material obtained from laboratory experiment it was 30.98°±1.71° for repose angle and 40.82°±3.21° for drawdown angle. In DEM simulation, the results were 0.892 for static friction coefficient and 0.269 for rolling resistance, generating a result of 30.10°±0.80° of repose angle and 42.31°±1.40° of drawdown angle.

5. Conclusions
The results produced by computational models depend strongly on what input values are used, which is why it is necessary to develop a calibration methodology. In this research it is proposed a methodology with 3 important stages and two types of models: experimental and DEM simulations.

The first stage corresponds to prepare the experimental procedure and the DEM simulations. This stage is essential because it lays the foundation for the experimentation and the research to achieve a good calibration process. In the second step we develop the experiment and the simulations. And in the last stage it is optimize the numerical parameters of the simulation, which best represent the behavior of the measurable variables in the experiment.

Regarding the results of calibration methodology proposed in this research, it is recommended:

- Chickpeas: a value of 0.18 for static friction coefficient, 0.94 millimeters of adhesive distance and 0.105 of rolling resistance.
- Copper sulfide ore: a value of 0.892 for static friction coefficient and 0.269 of rolling resistance.

Some of the important aspects to consider when carrying out the calibration methodology are the simulation time, the number of numerical parameters, the measurable variables and therefore the experiment.

Finally, the validation of the proposed methodology presented in this research should be done. For this, it is suggested to apply the methodology for the same granular material, using two different experiments and/or response variables, calibrating the same numerical parameters. If the optimized values of the parameters are similar, the methodology can be accepted as validated.

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