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DEM calibration approach: orthogonal experiment

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Abstract. The research considers conducting orthogonal experiment (OT) as one of the stages in developing a new discrete element method (DEM) parameters calibration approach. The measured responses in experiment are the parameters obtained by DEM animation processing using machine vision system (MVS). The variable factors in experiment are DEM parameters. A brief overview of an existing calibration approaches given in the article. The choice of OT as a design of experiment tool among other mathematical tools discussed. Experiments conducted using specially developed rig where bulk material's flow captured as DEM animation. DEM animation converted to video and then processed using MVS that allow register the values of such parameters as angle of repose or expiration time (measured responses). The results of the OT show that it is possible to identify four measured responses with the most valuable correlation coefficient. DEM parameters with the biggest influence on the measured responses identified for each of the obtained regression. Obtained results are useful in learning or iterative algorithms development for DEM parameters calibration.

1. Introduction

Discrete Element Method (DEM) is the most popular tool for the numerically calculating a large number of individual particles (bulk materials). DEM is used in various applications to optimize equipment in the mining and metallurgical or chemical industries (often used in integration with Computational Fluid Dynamics and Finite Element Analysis) [1–4, 21].

Despite the increasing popularity of DEM software before simulation starts users question what data about their bulk material should be implemented in the model. If parameters such as Poisson's ratio, Young's modulus and Density can be easily measured directly, then disagreements arise when matching static and dynamic friction coefficients or coefficient of restitution. The selection of such coefficients values which would provide appropriate rheological characteristics of simulated bulk material is called DEM parameters calibration [5-6].

DEM parameters calibration approaches are divided in to three groups: Direct Measurement Approach (DMA), Bulk Calibration Approach (BCA), and combined approach [7]. The principle of DMA is to measure all of the DEM parameters directly. The main problem with this approach is that each of the coefficients must be measured for an individual particle which could have different shapes and sizes within one bulk material [8]. This method is often used when simulating particles with the same shape and size (for example, in pharmacology [9]). Usually, a series of experiments are carried out and the results of the experiments are then averaged. In addition, the resulting coefficient values do not necessarily ideally reproduce the bulk material rheology in the DEM software, since existing DEM models can not accurately take into account absolutely all physical phenomena [10].

Very often, when integrating with DMA or separately, BCA is used to obtain appropriate values for DEM parameters. The BCA principle consists in iterative or algorithmic comparison of coefficients. The series of experiments stopping criteria is the achievement of proper rheological characteristics of the material. It means that characteristics obtained during experiment in the field as closely as possible matches the simulation results. Currently, this approach is actively developed by many researchers. Some of them offer conceptual solutions for accelerating the iterative matching of parameters [11–12], other use Generic Algorithms (GA) or Neural Networks (NN) to obtain DEM parameters [13, 15].

Another approach is to conduct the plan of experiment (PE) to determine the mathematical model of the measured response (for example, the angle of repose) from the varying DEM parameters. This approach is often used in the calibration of DEM parameters for bulk materials with certain physico-mechanical properties [16-17]. Moreover, a lot of researchers offer their own conceptual approaches [18–19, 14], based on this approach.

The original idea of this research is to conduct orthogonal experiment (OE) to determine a regression model, where the DEM parameters are the variable factors. The measured responses are the parameters obtained by DEM animation processing using the machine vision system (MVS) [22]. The choice of OE is justified by the fact that seven parameters variation at three levels guarantees the number of experiments equal to 2187. Conducting such number of experiments requires considerable computing power. The OE, however, makes it possible to conduct a second-order plan with the number of experiments equal to 143.

2. Mathematical model

Orthogonal experiment is a second-order plan. The main difference between the second-order and first-order plans is that when determining the regression, a quadratic influence of the varied factors on the response is taken into account. The design of experiment with factors x1 and x2 in figure 1 cannot consist only of experiments 1, 2, 3, 4 located at the vertices of the square of the PE 2^2 as it was for the first-order model. Experiments (star points) 5, 6, 7, 8 located on the axes x1 and x2 with coordinates (± α; 0), (0; ± α) and experiment 9 in the center of the square must be added to them. The purpose is that in any direction (5-9-6), (1-9-4), etc. there were three points determining the curvature of the surface in this direction. In the general case, the regression equation is:

$$y = b_0 + \sum_{i=1}^{k} b_i x_i + \sum_{i=1}^{k} b_{iu} x_i x_u + \sum_{i=1}^{k} b_i^{'} x_i^{'} \qquad (1)$$

where y – response, b_0 – nondimensional coefficient, b_i – the linear coefficient at the factor, k – the number of parameters, b_{iu} – coefficient of parameters paired influence, $b_i^{'}$ – coefficient parameters quadratic influence, x_i, x_u – the coded value of the factor, $x_i^{'}$ – the coded value of the quadric influence factor.

The regression's b coefficients are calculated according to well-known equations. The resulting regressions will contain information about the DEM parameters influence on the responses (for example, the angle of the repose) for a particular bulk material. It is possible to evaluate the possibility of using the measured response for DEM parameters calibration (with correlation coefficient).

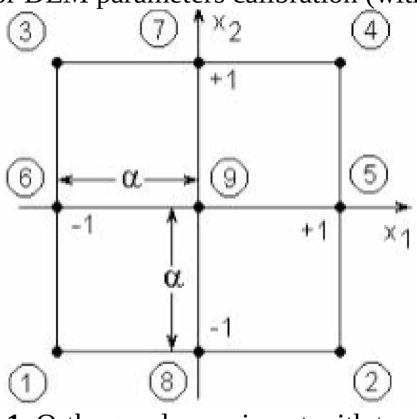

Figure 1. Orthogonal experiment with two factors

3. Experiment preparation

DEM parameters calibration approach using PE or OE involves conducting a series of experiments for bulk material with certain physical and mechanical properties. It was decided to simulate a gravel-like material with a spherical particles 8 mm diameter. The shape and diameter were chosen due to the simplification of the numerical calculation (selected bulk material is an example for the approach). In addition, the maximum particles diameter is limited by the size of the rig, which will be discussed later. A non-linear DEM model is selected for simulation. The remaining parameters of the bulk material are summarized in table 1.

Next step is to determine the variable factors. The factors are DEM parameters that require calibration. Since the simulated particles are spheres rolling resistance (RR) was also taken into account. All 7 calibrated parameters are summarized in table 2.

Specially designed rig (figure 2) was used in the experiments. The design of the rig assumes the presence of two removable dampers. After the first one removes the angle of rupture is formed and the after the second - the angle of repose. The walls of the rig are made of transparent plexiglas to make possible bulk material flow analyzing using a high-speed camera to capture the video [22]. The rig has a particles diameter limitation - no more than 10 mm to ensure particles free flow. 3D CAD model was loaded into Rocky DEM software [20] for numerical simulations. An example of the bulk material outflow and the angles of repose and rupture formation is shown in figure 3.

Table 1. Simulated bulk material parameters

Parameter	Value
Poisson's ratio	0.3
Young modulus	10^6 kPa
Density, kg/m^3	1300
Shape	sphere
Particle size distribution	100% 8 mm diameter
Contact model	Non-linear
Gravity acceleration	9.81 m/s^2

Table 2. **Calibrated DEM parameters**

Particle-Particle	Static Friction	Dynamic Friction	Restitution	Rolling resistance
Particle-Boundary	Static Friction	Dynamic Friction	Restitution	

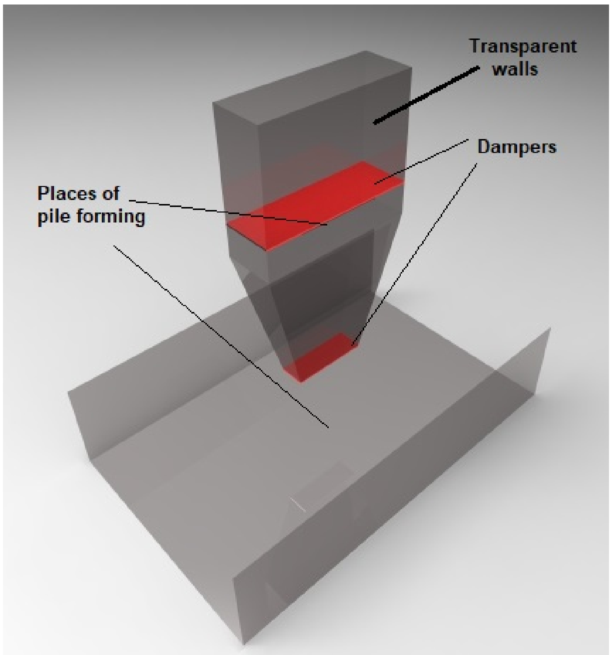

Figure 2. Designed rig

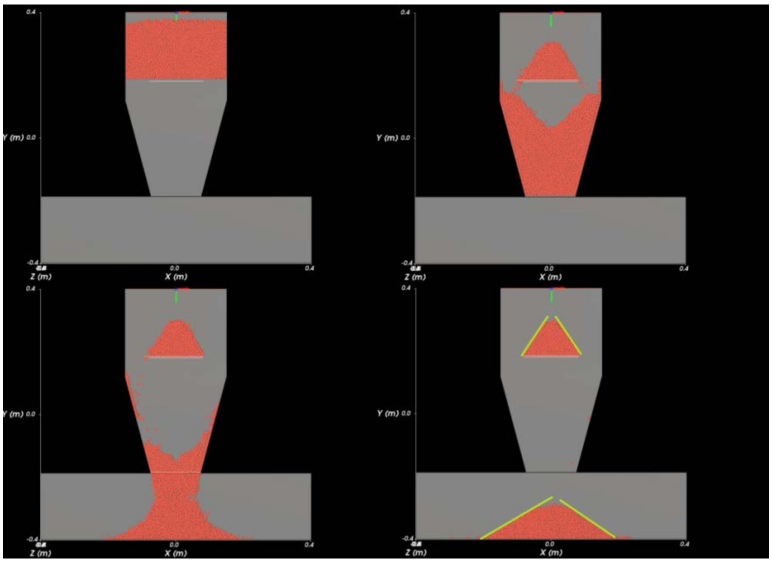

Figure 3. Bulk material simulation example

4. Experiment handling

First of all, we need to determine OE points for the DEM parameters (factors). The center point of the experiment is taken as 0.5 for each parameter. Accordingly, +1 - 0,65; -1 - 0.35; + α - 0,8; -α = 0.2. In the 143 experiments OE plan takes the form as shown in table 3.

The measured responses in experiments are the parameters obtained by processing the bulk material behavior DEM animation using a machine vision system. The rig design and image processing algorithms allow to extract up to 43 different parameters. However, among them, 4 most unique parameters were identified: the angle of repose and the angle of rupture (figure 4), the expiration time (figure 5) and the visual image "parabola" (figure 6).

Table 3. **Orthogonal experiment plan**

N	X_0	SFpp	SFpb	DFpp	DFpb	CoRpp	CoRpb	RR	SFppSFpb	…	SF’pp	…
1	+1	-1	-1	-1	-1	-1	-1	-1	+1	…	0,1	…
2	+1	-1	-1	-1	-1	-1	-1	+1	+1	…	0,1	…
3	+1	-1	-1	-1	-1	-1	+1	-1	+1	…	0,1	…
4	+1	-1	-1	-1	-1	-1	+1	+1	+1	…	0,1	…
5	+1	-1	-1	-1	-1	+1	-1	-1	+1	…	0,1	…
6	+1	-1	-1	-1	-1	+1	-1	+1	+1	…	0,1	…
7	+1	-1	-1	-1	-1	+1	+1	-1	+1	…	0,1	…
8	+1	-1	-1	-1	-1	+1	+1	+1	+1	…	0,1	…
9	+1	-1	-1	-1	+1	-1	-1	-1	+1	…	0,1	…
…	…	…	…	…	…	…	…	…	…	…	…	…
128	+1	+1	+1	+1	+1	+1	+1	+1	+1	…	0,1	…
129	+1	+α	0	0	0	0	0	0	0	…	-0,26	…
130	+1	-α	0	0	0	0	0	0	0	…	-0,26	…
131	+1	0	+α	0	0	0	0	0	0	…	-0,9	…
132	+1	0	-α	0	0	0	0	0	0	…	-0,9	…
133	+1	0	0	+α	0	0	0	0	0	…	-0,9	…
134	+1	0	0	-α	0	0	0	0	0	…	-0,9	…
135	+1	0	0	0	+α	0	0	0	0	…	-0,9	…
136	+1	0	0	0	-α	0	0	0	0	…	-0,9	…
…	…	…	…	…	…	…	…	…	…	…	…	…
143	+1	0	0	0	0	0	0	0	0	…	-0,9	…

The expiration time from the funnel is interpreted through the material's filling degree in the expiration area. The time origin is taken at the moment of the second damper removing. The end of countdown is when the value filling degree becomes less than 4% (the threshold is obtained empirically). The visual image "parabola" is obtained by image filtration and extracting the points contour on a fixed frame in each experiment. The resulting contour is approximated in the parabola equation $y = ax^2+bx +c$ by the least squares method. Thus, it is possible to extract up to 3 parameters: the parabola coefficients a, b and c.

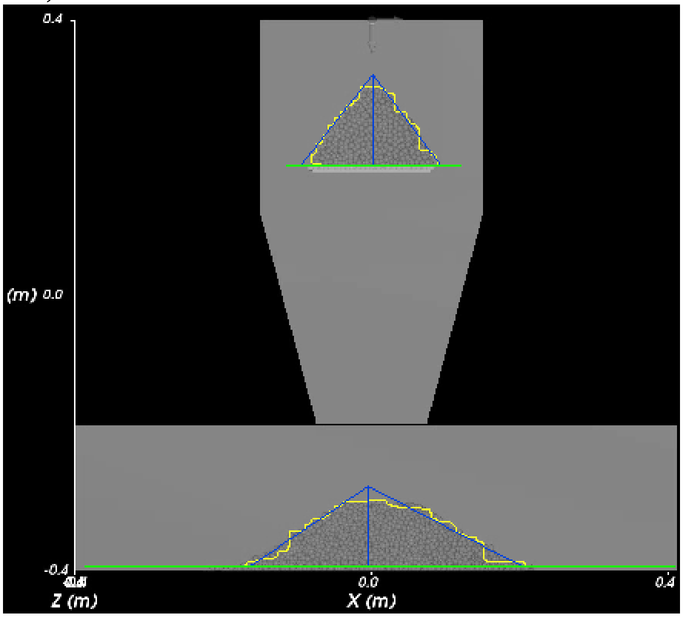

Figure 4. Angles of rupture and repose interpretation

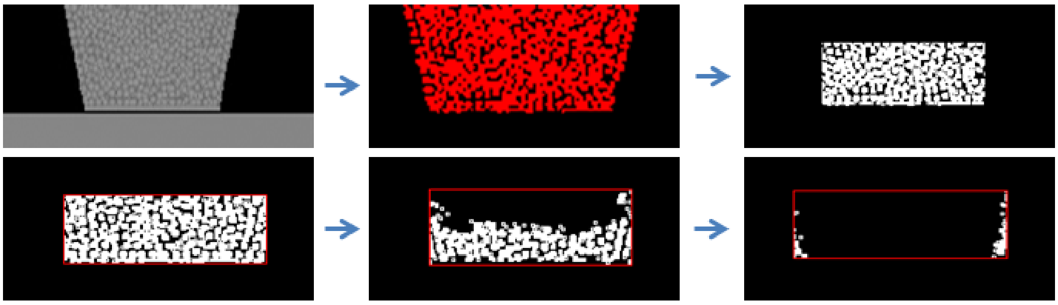

Figure 5. Expiration time interpretation

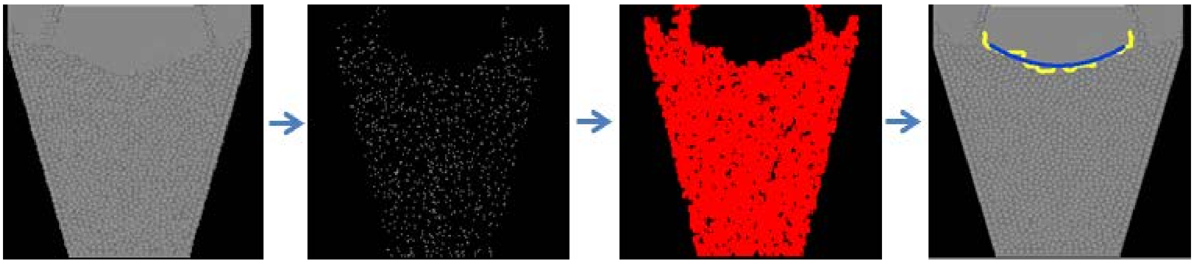

Figure 6. Visual image "parabola" interpretation

5. Experiment results

Six regression dependences of the form (1) between the DEM parameters and the measured responses (the angles of repose and rupture, the parabola coefficients a, b and c, and the expiration time) were obtained by results of experiment. The correlation coefficient and the mean error between the experimental and model values of the response were calculated for each of the regression. The correlation coefficients for each of the regression are shown in table 4.

It is quite obvious that the coefficients of parabola b and c are not of any interest. The values of these coefficients as measured responses do not practically change from the DEM parameters variation, which leads to low correlation coefficients values for the regressions. The remaining 4 parameters have a high correlation coefficient values and show a very high (angle of repose) and high (remaining) bonding. Figure 7 graphically demonstrates the distribution of the experimental and model responses values for all the experiments.

As can be seen in fig. 7 the points field for each of the dependencies almost exactly lies at 45^0 angle, which indicates the absence of a static error and any disturbance is random. The average deviation (error) between the experimental and model responses values are given in table 5.

Table 4. Correlation coefficients for the obtained regressions

Response	Correlation coefficient
Angle of repose	0.903
Parabola A	0.816
Expiration time	0.794
Angle of rupture	0.725
Parabola B	0.474
Parabola C	0.223

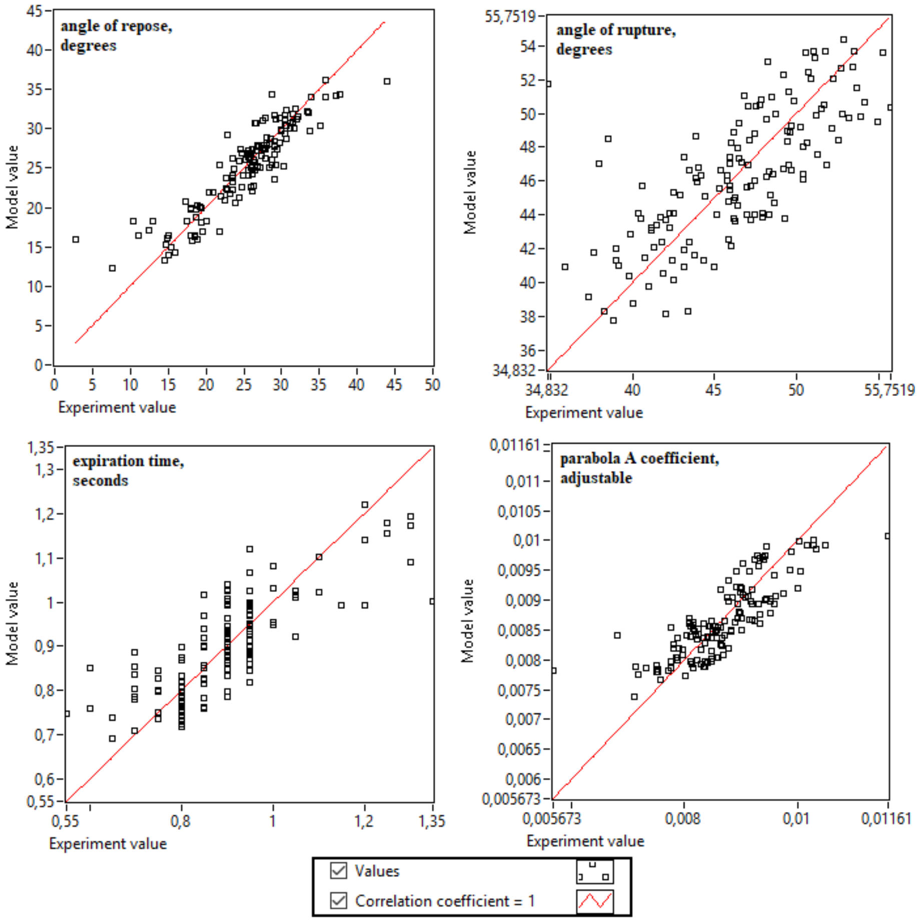

Figure 7. Graphical interpretation of experiment and model values distribution

Table 5. Average error between experiment and model response values

Response	Error, %
Angle of repose	1,13
Parabola A	0,15
Expiration time	0,41
Angle of rupture	0,24

Table 6. DEM parameters influence on the measured responses

Response	DEM parameters influence in descending order (from left to right)						
Angle of repose	DFpb	RR	DFpp	CoRpp	SFpp	CoRpb	SFpb
Parabola A	RR	DFpp	SFpp	CoRpp	SFpb	DFpb	CoRpb
Expiration time	DFpb	DFpp	RR	SFpp	CoRpp	CoRpb	SFpb
Angle of rupture	RR	SFpp	CoRpp	DFpp	DFpb	CoRpb	SFpb

The average error values are almost equal to 0, which indicates a random error distribution in all experiments and absence of the methodological error. This means that the error value does not depend on the geometry of the developed rig or on the applied image processing algorithms.

The regression's b coefficients help to evaluate the influence degree of the variable DEM parameters on the measured responses. DEM parameters, sorted in descending order of the coefficient b value for each of the responses, are presented in table 6.

In all cases, rolling resistance has a strong influence on responses, which is an expected result, because experiments were held with spherical particles. In addition, there is a noticeable difference between the angle of repose and rupture. For the angle of rupture static friction is more important parameter than dynamic and for the angle of repose dynamic friction has stronger influence rather than static. There is also a general trend of a particle-particle interaction higher influence than particle-boundary. This means that the behavior of bulk material is more dependent on the interaction between the particles than on the interaction between particles and the surface (boundary).

6. Conclusion

Conducting orthogonal experiment where the variable factors are DEM parameters, and the responses are parameters measured by machine vision system, gives a lot of useful information that can be used in developing new DEM parameters calibration approach. Obtaining regression dependencies and evaluating its adequacy with correlation coefficient identifies responses that can be applied in learning algorithms (machine learning or generic algorithms). For experiment conducted in this research such parameters are the angles of repose and rupture, expiration time and the "parabola" coefficient A. In addition, DEM parameters influence on measured responses data can be applied in iterative algorithms where calibration is performed by blind DEM parameters variation. As an example to achieve the desired angle of repose, you should start variation form dynamic friction for particle-boundary interaction and rolling resistance (if simulating spheres), since they exert the strongest influence on the angle of repose.

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