The 7th International Conference on Discrete Element Methods
August 1 to August 4, 2016
Dalian, China

Verification of an automated work flow for discrete element material parameter calibration

Rackl, Michael[1]; Hanley, Kevin J.[2]; Günthner, Willibald A.[1]

Abstract. Identification of parameter values for discrete element method (DEM) material models is a major issue for realistic simulation of bulk materials. Choosing suitable parameter values is often done using trial and error in a disorganized manner, where efficiency largely depends on the experience of the DEM user. A methodical work flow, which is based on Latin hypercube sampling, Kriging and numerical optimization, was composed with open-source software. The calibrated DEM materials were subsequently validated against the physical data from measurements and the number of required DEM simulations was recorded to assess the effectiveness of the overall method. The simulation results were within a few percent of the desired experimental values after an average of 14 DEM runs. Disadvantageous boundary conditions, like a wide factor value range or the optimum being located at an edge, did not considerably influence the quality of the results.

Keywords: calibration; Kriging; Design of Experiments (DoE); optimization

1 Introduction

The discrete element method (DEM) has gradually gained acceptance as a useful tool for predicting the behaviour of bulk particulates. One factor which has inhibited the adoption of DEM is the difficulty in choosing suitable input parameters for the simulations, particularly those parameters which are not easily related to physical measurements of the material, e.g., interparticle friction coefficient. Most DEM simulations contain some parameters which can be obtained only by calibration, i.e., by varying the unknown simulation parameters until the simulation results are in good agreement with equivalent physical measurements. Some efforts

[1] M. Rackl (✉)
Institute for Materials Handling, Material Flow, Logistics; Technical University of Munich, Boltzmannstrasse 15, 85748 Garching, Germany; e-mail: rackl@fml.mw.tum.de

[2] Institute for Infrastructure and Environment, School of Engineering, The University of Edinburgh, Edinburgh EH9 3JL, United Kingdom

have been made to establish robust methods for DEM calibration, e.g., Yoon (2007), Favier et al. (2010), Johnstone (2010), Benvenuti at al. (2016). However, these are not widely used and *ad hoc* trial-and-error methods remain predominant which have many disadvantages (Hanley et al., 2011).

An automated workflow for DEM material model calibration was described by Rackl et al. (2016). The DEM code used for this demonstration was LIGGGHTS (Kloss et al., 2012), the methodology was based on Latin hypercube sampling (LHS), Kriging and numerical optimization, and the simulations were planned and controlled using GNU Octave (Eaton et al., 2015). The aim of this paper is to verify the capability and efficiency of this approach for calibrating contact law parameters based on physical measurements of the angle of repose and bulk density.

2 Materials and Methods

The calibration process, described in Section 2.1, was verified by comparing its resulting solution sets against reference results from the same DEM model (described in Section 2.2). The numerical experiments and reference results are described in Sections 2.3 and 2.4, respectively.

2.1 Calibration Method

The calibration method applied in this study was described in detail by Rackl et al. (2016). In summary, it uses a two-step optimization process implemented in Octave (Eaton et al., 2015). The first optimization step is based on a Kriging meta model, which is parameterized with response data from sample points of a DEM model for the angle of repose and bulk density. Sample points are generated by means of Latin hypercube sampling (LHS). The user-defined material and contact parameter values are varied to obtain the required response data. Then multi-objective optimization is applied to the Kriging models using a non-linear residual minimization approach based on the Levenberg-Marquardt algorithm (Levenberg, 1944; Marquardt, 1963). The specified multi-objective cost function includes the relative difference between physical measurements of the angle of repose and bulk density and a criterion involving the Rayleigh time step size. The latter is included to penalize choosing computationally-expensive sets of DEM parameters. In the second step, optimized material parameter values of the particle density and rolling friction from the Kriging models are then used as starting values for the second optimization process. The latter optimizes the parameters using the actual DEM model.

2.2 DEM Model

This study used a simple DEM model to generate results for the bulk density and angle of repose. It consists of a top- and bottomless cylindrical steel container, placed onto a steel plate. In a first step, the cylindrical container is filled with particles, up to a certain height, so the bulk density can be measured using the known volume and mass within. In a second step, the container is lifted up, so the particles lose their lateral support and start forming a heap. From this heap, the angle of repose is measured using image processing. The DEM code used was LIGGGHTS. A Hertz-Mindlin contact model was used with an elastic-plastic spring-dashpot (EPSD) rolling friction model.

2.3 Numerical Experiments

Solution sets for various combinations of boundary conditions were generated. The factors and factor levels were selected based on the expected usage of the calibration process, where a DEM user estimates DEM contact model parameters and knows the approximate interval in which the most suitable parameter values are likely to occur.

2.3.1 Factors and Factor Levels

The robustness of the calibration method described in Rackl et al. (2016) was to be tested against four factors. With regard to the intended use of the calibration method, two of them can be viewed as stochastic, whereas the other two are based on human decisions.

The last two factors, i.e., those which can be actively chosen, are the factor interval width (FIW, in percent) and the number of sample points that are used to generate input for the Kriging models. In the progress of this study, the latter is expressed based on the number of factors used for the calibration process (samples per factor, samPfact). The FIW determines the range for each of the parameters to be used for calibration, i.e., FIW=33% yields a parameter range from 67 to 133 for a centered layout taking 100 as the base value. The two factors of stochastic nature are the random seed of the DEM particle factory in LIGGGHTS (rndSd) and the location of the optimal parameter set for the given DEM model (locOpt). The location is expressed in relation to the factor interval boundaries used for the calibration parameters.

Three situations can be thought of for this location. Firstly, the optimal solution set lies right in the center of the calibration factor space. This situation would be ideal in terms of the optimization and only occurs when the user's initial guess for the parameters is optimal by chance. Secondly, the optimum lies inside the boundaries of the factor interval space, but is not in the center. This is considered most common, since the initial guess may not be exactly correct but at least within a sensible range of the optimum. Thirdly, and least favorably, the optimum for at least one of the calibration factors lies outside of the user-specified factor interval space. In this case the calibration method may output that the corresponding factor is located at the maximum or minimum value of the interval. If such a result is obtained, the choice of factor interval has to be adapted and the calibration process repeated. For this study, two locations were studied. These are (1) at the center and (2) at the corner where all calibration factor values are minimal. The factors and factor levels used in this study are listed in Figure 1.

2.3.2 Experimental Plan

The experimental plan used for the numerical experiments in this study was created and evaluated with R (R Core Team, 2014) and the package RcmdrPlugin.DoE (Groemping, 2014). It is a full-factorial design containing two two-level factors and two three-level factors, consisting of 36 distinct combinations of factor levels. Each run was repeated three times to be able to estimate the variance of the results as well as the repeatability of the calibration method. Figure 1 schematically shows the experimental plan without repeat runs.

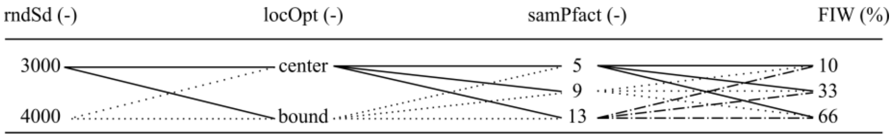

Figure 1: Schematic overview of factors, factor levels and all 36 factor combinations.

2.4 Reference Results for the Calibration Process

For verification of the calibration process, the DEM model described in Rackl et al. (2016) was used as a reference. As in this paper, particle density and rolling friction coefficient were used to calibrate the angle of repose (AoR) and bulk density (BD) based on data from literature. The DEM model was investigated at 400 sample locations, based on an evenly-spaced regular 20x20 grid for the density and rolling friction. Results for the AoR and the BD were recorded and used to parameterize two Kriging models. Based on these Kriging models, surface plots were created for both the AoR and BD. They were subsequently used to find parameter combinations of rolling friction and density which yield results within a span of ±5% of the desired AoR and BD of 22° and 1500 kg/m^3. The intersection of both of these parameter sets was then considered to be the expected output of the calibration process.

3 Results and Discussion

The majority of solution sets were in excellent agreement with the expected outcome and desired values for the angle of repose and bulk density were closely matched.

3.1 Reference Results

The reference models for the angle of repose and the bulk density are based on 400 samples from the DEM model. The resulting contour plots are depicted in Figure 2.

An angle of repose of 22° is somewhat hard to obtain with the selected model. As Figure 2a shows, the lower the particle density and the higher the rolling friction, the higher the angle of repose becomes. The bulk density scales almost linearly with the particle density. Nonetheless, it reaches a plateau at particle densities greater than 2500 kg/m^3. Rolling friction does not considerably influence the bulk density in this model.

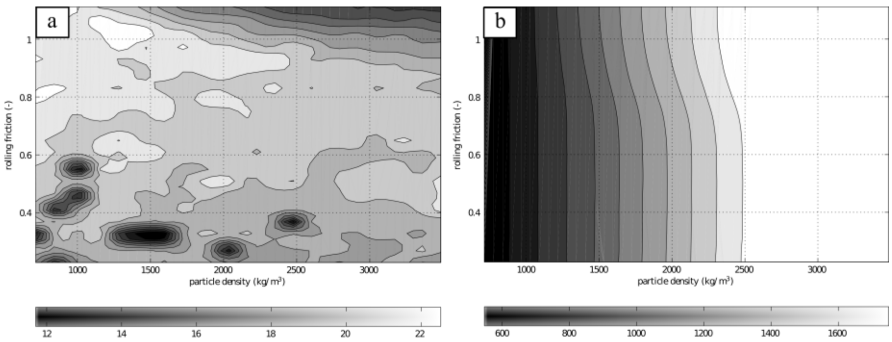

Figure 2: Contour plots for the angle of repose (a) and bulk density (b), based on the reference models. Units are (°) and (kg/m^3), respectively.

In Figures 3a and 3b, the desired 5% span is depicted for the angle of repose and bulk density. Figure 3c shows the intersection of both solution spaces. It can be seen how combining additional desired results reduces the diversity of possible solutions. However, there still exists a broad range of solutions, especially for the rolling friction, which could be approximately 0.5 or 0.7 to 1.

3.2 Calibration Process Results

The calibration process functioned robustly and yielded results within the expected solution space. A small percentage of solution sets was located at greater distances from the expected outcome; these sets were investigated in more detail.

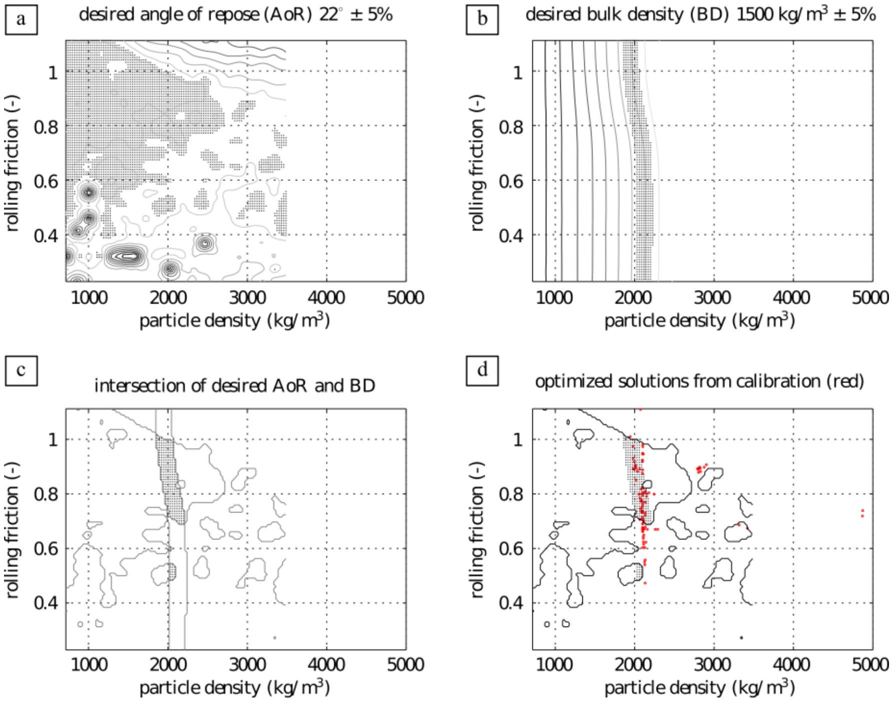

Figure 3: Desired AoR and BD solutions (±5% span) are indicated by black dots (a, b, c). Figure (d) shows the location of obtained solution sets in red.

3.2.1 General Findings

From all 108 calibration runs, 93 (~86%) resulted in a parameter set which lay within or close to the expected areas (termed 'main', Figure 3d). This shows that the calibration process gave sensible results for most of the cases tested in this study. Desired angle of repose and bulk density values were matched with mean differences of 1.7% (min. 0%, max. 18%) and 5% (min. 0%, max. 24.5%), respectively. It took the calibration process an average of 14 runs (LHS excluded, min. 8, max. 37) to obtain a solution set and each set was reported back as "converged" from the optimization algorithm. From the rest of the obtained solution sets, 11 (10%) were in a cluster located around an optimized density (ρ_O) of 2824 kg/m^3 ('island'). Two further groups with two members each (1.9%) were at ρ_O around

3368 (‘isle_m’) and 4871 kg/m^3 (‘isle_r’), respectively. Corresponding mean values for the different categories of results are listed in Table 1.

Table 1: Mean values for the three result groups from the calibration process.
ρ_O: optimized particle density; $\mu_{r,O}$: optimized rolling friction coefficient

group	**no. of solution sets in group**	**AoR** (°)	**BD** (kg/m^3)	$\boldsymbol{\rho_O}$ (kg/m^3)	$\boldsymbol{\mu_{r,O}}$ (-)
main	93	21.7	1521	2096	0.76
island	11	21.9	1868	2824	0.89
isle_r	2	21.9	1867	4871	0.73
isle_m	2	21.9	1868	3368	0.68

3.2.2 Remote Solution Sets from the Calibration Process

Closer examination of the island solution group showed that each of the 11 sets was a result from the factor combinations locOpt=bound and FIW=33%. The two sets of isle_r were both results from rndSd=4000, locOpt=bound, samPfact=13 and FIW=66%. The results in isle_m had samPfact=9, rndSd=4000 and locOpt=bound in common.

All of the results located outside of the expected solution region resulted from runs where the expected solution is located at the minimum values of the calibration factor interval (locOpt=bound). The lower density interval boundary for all configurations with locOpt=bound was 2100 kg/m^3: very close to the computed main area results in the ‘main’ group. This means that the residual of the Rayleigh time step will always be around 1 for the expected solution area. Thus, any test run with the locOpt=bound tends to seek an optimal solution where the particle density (and hence the time step) is larger. It can be seen from Table 2 that with locOpt=bound each of the remote result groups gave a lower sum of residuals than the main group. It can be concluded that the initial selection of the factor interval width, in combination with an unexpected “optimal” solution location can lead to undesirable results, where measurement data are neglected in favour of a larger Rayleigh time step. It is unclear how this effect affects the calibration process results, when more parameters which alter the Rayleigh time step are included for calibration, e.g., Young’s modulus which could considerably affect the time step.

4 Conclusion and Outlook

The results of this study showed that the automatic DEM material model calibration process described in Rackl et al. (2016) is capable of robustly identifying suitable contact law parameters to fit physical measurements for the angle of repose and bulk density, under various boundary conditions. Involving the time step in the optimization process helps the algorithm to select efficient contact law parameters.

Future studies should include more factors for calibration of the contact law parameters and add more DEM models to calibrate. Besides particle density and rolling friction, parameters such as Young's modulus and static friction coefficients could be added to increase the degrees of freedom the optimization algorithm can process. One would then be truly able to evaluate the usefulness of this approach, since the state-of-the-art approach for calibration of DEM parameters is trial-and-error and human calibrators are very likely to lose track of the calibration process; this is especially true when many factors and several DEM models are involved.

Table 2: Residuals (10^{-2}) and residual sums (in brackets) of the optimization algorithm. Residual sums are computed as sum of the absolute terms of AoR, BD and the corresponding Rayleigh time step (RLTS) portion; mean values were used for each group. Note that a multi-variate optimization algorithm is used for the calibration process (cf. Rackl et al. (2016)).

residual for	**main**	**island**	**isle_r**	**isle_m**
AoR	−1.4	−0.86	−0.68	−0.68
BD	1.4	24.5	24.5	24.5
RLTS, 10%	100 (103)	-	-	-
RLTS, 33%	100 (103)	44.6 (70.0)	-	7.6 (32.8)
RLTS, 66%	100 (103)	69.5 (94.9)	0.03 (25.2)	49.1 (74.3)

5 References

Benvenuti L, Kloss C, Pirker S (2016) Identification of DEM simulation parameters by Artificial Neural Networks and bulk experiments. Powder Technol 291: 456–465

Eaton JW, Bateman D, Hauberg S, Wehbring R (2015) GNU Octave version 4.0.0 manual: a high-level interactive language for numerical computations

Favier J, Curry D, LaRoche R (2010) Calibration of DEM material models to approximate bulk particle characteristics. Proc. 6th World Congress on Particle Technology, Nuremberg

Groemping U (2014) RcmdrPlugin.DoE: R Commander Plugin for (industrial) Design of Experiments (computer software)

Hanley KJ, O'Sullivan C, Oliveira JC, Cronin K, Byrne EP (2011) Application of Taguchi methods to DEM calibration of bonded agglomerates. Powder Technol 210(3): 230–240

Johnstone M (2010) Calibration of DEM models for granular materials using bulk physical tests. PhD thesis, University of Edinburgh

Kloss C, Goniva C, Hager A, Amberger S, Pirker S (2012) Models, algorithms and validation for opensource DEM and CFD-DEM. Prog Comput Fluid Dyn 12(2/3):140–152

Levenberg K (1944) A method for the solution of certain non-linear problems in least squares. Q Appl Math 2: 164–168

Marquardt DW (1963) An algorithm for least-squares estimation of nonlinear parameters. J Soc Ind Appl Math 11(2):431–441

R Core Team (2014) R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna

Rackl M, Görnig CD, Hanley KJ, Günthner WA (2016) Efficient Calibration of Discrete Element Material Model Parameters using Latin Hypercube Sampling and Kriging. Proc. ECCOMAS 2016, Crete Island, Greece (accepted paper)

Yoon J (2007) Application of experimental design and optimization to PFC model calibration in uniaxial compression simulation. Int J Rock Mech Min 44(6): 871–889