Framework for DEM Model Calibration and Validation

Johannes Quist, Magnus Evertsson

Chalmers Rock Processing Systems
Department of Product and Production Development, Chalmers University of Technology, SE-41296 Göteborg, Sweden
johannes.quist@chalmers.se

Abstract. The discrete element method (DEM) is used for modelling and simulating particle flow behaviour in research and industrial applications. If the results from such a simulation are to be trusted in a research project or be used as knowledge basis in engineering decision making, the modeller will need to apply some kind of calibration and validation approach. Even though most researchers and engineers apply some kind of method for calibration of the model and validation of the results, no general consensus or calibration methodology framework has been established that governs the quality or accuracy. DEM simulations are now used for modelling a vast number of machines and processes in minerals processing. It is hence of essence that the academia and industry continues the process of discussing a methodology for calibrating rock and ore materials. This paper aims at joining this discussion by presenting a general framework. The approach is based on the calibration framework proposed by Hofmann (2005) and adopting it to calibration of DEM models.

The framework is based on calibration and validation on three different levels ranging from the basic single contact model parameter calibration; to a mid-level flow property test; to a full scale experiment. A calibration device has been developed in order to facilitate multiple flow regime experiments with directly observable particle flow paths. In order to efficiently perform both calibration experiments and simulations a design of experiments approach is applied. The actual calibration is conducted by minimizing the error between the experimental domain and the simulation domain by applying multi-objective optimization methods.

Keywords: DEM, Calibration, Validation, Simulation, Modelling,

INTRODUCTION

When applying the discrete element method for simulating particle flow behaviour in research or industrial applications it is vital to have a robust approach in regards to validation and calibration of the models. Material, contact model (e.g. the Hertz Mindlin contact mode, see Figure 1) and simulation parameters need to be chosen in such a way that the resulting particle flow behaviour corresponds to a realistic performance. This is commonly done by conducting multiple simple experiments such as a slope test where outputs such as repose angle are matched between experiment and simulation.

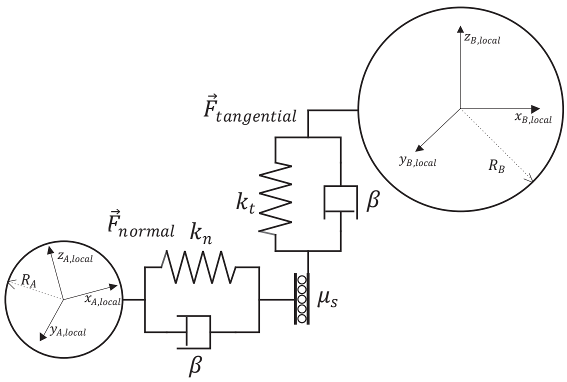

Figure 1. Schematic illustration of the Hertz Mindlin contact model

As previously mentioned it is important to make sure that the DEM models and simulations conform to the realistic behaviour of rock material. Otherwise it will be difficult to utilize DEM as a viable tool for decision making. In Figure 2 the concept of the V-model for DEM calibration and validation is presented. The V-model is known within the field of product development as an approach for decomposition of product system architecture on the left leg and a corresponding decomposition of requirements on the right leg. In this version the left leg corresponds to the experimental domain and the right leg to the simulation and modelling domain.

There are several researchers who have targeted the topic of DEM and calibration. Coetzee (Coetzee, 2009; Coetzee and Nel, 2014), Grima and Wypych (Grima, 2011), Gröger (Gröger, 2006), González-Montellano (González-Montellano et al., 2011), Combarros (Combarros et al., 2014), Barrios (Barrios et al., 2013), Frankowski (Frankowski and Morgeneyer, 2013) and Favier (Favier, 2010) have all made important contributions in the area of contact model parameter calibration for particle flow applications. In the area of calibrating bonded particle models, Hanley (Hanley et al., 2011), Yoon (Yoon, 2007), Wang (Wang and Tonon, 2009) have made vital advancements.

In the literature, the calibration of DEM model parameters is commonly approached by conducting single property laboratory tests. This could e.g. be a particle bounce test to calibrate the coefficient of restitution or a particle sliding test to determine the coefficient of static friction. While this is an important step it is only the first level of calibration. The single property at a time approach does not guarantee that the particle population behaves according to the real material behaviour.

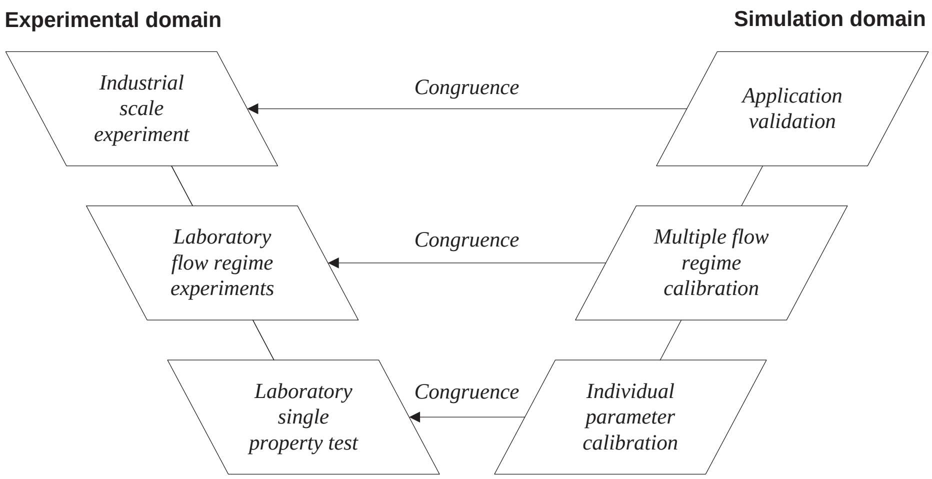

Figure 2. Proposed V-model for DEM calibration and validation

The second level calibration based on multiple flow regime experiments is needed in order to make sure that the aggregated behaviour of all model parameters demonstrates an agreement in a good correspondence within a stipulated range of accuracy. The validation on the top level in conducted on the application level, by comparing simulation outcome with actual scale experimental data.

According to the terminology and framework proposed by Schlesinger et al (Schlesinger, 1979) validation may also be done in regards to the conceptual model of a system.

1.1 Calibration Device

A new device has been designed and built for the purpose of contact model calibration of granular material. An illustration of the device can be seen in Figure 3. In order to be able to measure several flow properties in the same experiment the device is built up by different features. Each feature can be individually adjusted in order to create different flow regimes. The experiment is conducted in the following sequence:

i. Hopper angle, sliding plane angle and top section height is adjusted
ii. The material sample is placed in the hopper
iii. High speed camera is triggered ON
iv. Trap door mechanism released
v. Material flows through hopper
vi. Material slides on sliding plane
vii. Material bounces on left wall
viii. Material settles forming a sloped bed
ix. High speed camera triggered OFF
x. Repose angle of sloped bed is manually measured
xi. Material is discharged

The flow passing through the device can be monitored directly due to the transparent front glass sheet. In Figure 4 an example of the flow in the experiment and the corresponding flow in the simulation are shown. As the figure indicates it is possible to subjectively make a judgement if the simulated material flow and behaves in the same way as the experiment. However, a subjective judgement is not good enough if the objective is to calibrate the model in a more strict sense. The response variables measured from the experiment is the mass flow through the hopper and the repose angle of the bed formation. An example of a bed formation is shown in Figure 5.

Figure 3. Illustration of the calibration device

Figure 4. The left hand side image shows a frame from a recording of a real experiment after the first stream of particles have travelled through the device. The right hand side image shows the corresponding flow in the simulation environment.

A high speed camera is also used to capture the flow for further analysis using motion tracking. This gives the possibility to measure the actual flow pattern of particles, not only indirect bulk flow properties. Guiding experiments shows that colour-marked particles can be tracked as part of the bulk material. Six particles have been marked and positioned in the same pattern for each flow experiment.

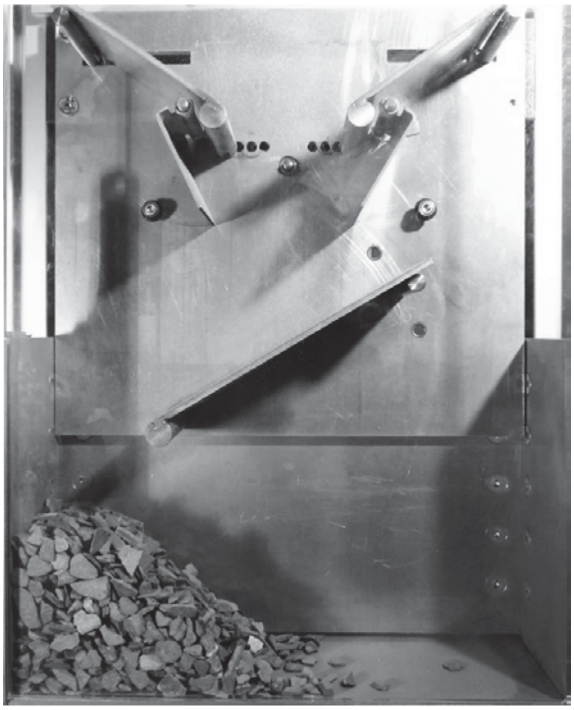

Figure 5. Image of the repose angle formation at the end of a flow experiment.

In Figure 6 an example of particle flow profiles in the x- and y-direction is presented. The red and blue colour represents two different flow regime settings and the particles tracked are placed in the same position at test initiation.

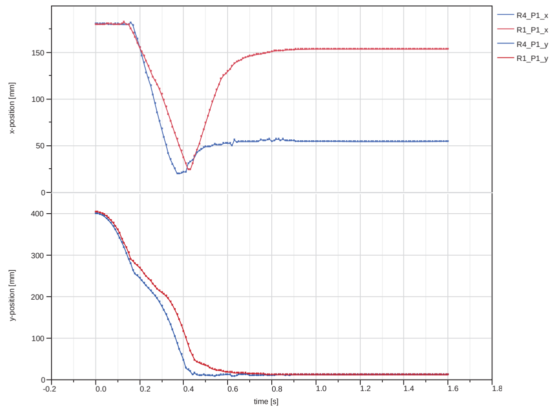

Figure 6. Example of motion tracking data showing x- and y-coordinate positions during the flow for a marker particle with the same starting position.

The particles tracked in the plot are placed cantered on top of the trap door latch. The particle route through the device can be described as a sequence as seen in Table 1. The experiment represented by a blue line (R4) in the plot has a flow regime setting with a steeper sliding plane angle than the red line experiment (R1).

Table 1. Flow sequence of marker particle in Figure 6 through the device.

Seq.	Time [s]	Description
1	0 – 0.16	Free fall flow out of the hopper
2	0.16 – 0.4	Particle slides on the sliding plane
3	0.4 – 0.8	Particle bounces on the left wall and settles in the pile formation
4	0.8 – 1.6	Particle is settled

The developed method for direct measurement of the particle flow is promising and gives a good subjective understanding. However, so far the method has not been developed far enough to enable a statistical comparison to simulation data. A higher level of automated data analysis for both motion tracking trajectory data and simulation trajectory data is needed in order to compare the experimental and simulation domains.

Calibration Framework

Model calibration is essentially the process of adjusting model parameters in order to comply with a reference system. The reference system is either experimental data or a higher fidelity model. When performing calibration of any numerical model the question arises; *under what conditions may a model be considered as calibrated?*

Hofmann (2005) has proposed a formal definition for this problem. A schematic diagram of the calibration framework can be seen in Figure 7. The framework consists of a model domain and a reference system domain. The set of possible model input values is denoted as X^M for the model and X^S for the reference system. The reference system dynamics function φ^S gives the possible values of the reference system output Y^S. The model transformation function φ^M controls the model output Y^M given a set of model parameters P^M. The model parameters P^M are the subject of the calibration exercise. According to this system a model and reference system is simplified to its input, output and the transformation between them. In addition, Hofmann defines the assumption that the input of the reference system (X^S) can be transformed into the input of the model (X^M) and that the output of the model (Y^M) can be (re-) transformed into the output of the reference system (Y^S) by invertible functions $\psi : X^S \to X^M$ and $\omega : \mathrm{Y}^M \to Y^S$.

A model is said to have *weak congruence* if for every possible system input there exists at least one parameter configuration of the model, so that the outcome of the model application equals the output of the system. The definition of a *strong congruence* denotes that there exists at least one model parameter configuration so that for all possible system inputs the outcome of the model application equals the output of the reference system.

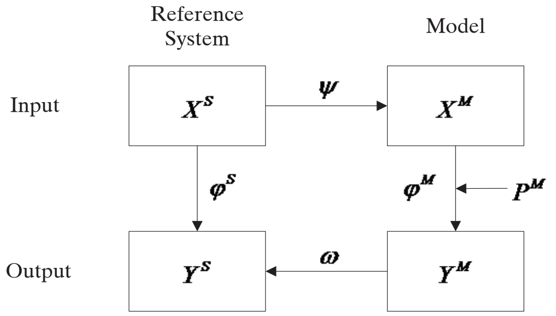

Figure 7. Model calibration framework (re-drawn from (Hofmann, 2005))

If the model exhibits weak congruence the model parameters need to be adjusted for every new model application. Hence it serves poor value as the model is not usable when moving from the laboratory experiment to the industrial application.

The definition of strong congruence states that if the model is calibrated on one model application it will be true for all others. This condition is highly unlikely in the case of complex DEM simulation applications and the definition is also impractically rigid in the mathematical equality notation. As a remedy to this problem Hofmann proposes the concept of *pragmatic congruence* where the model application and reference system is judged in regards to a problem specific tolerance deviation ε_j. The definition of pragmatic congruence is written in Eq. (1).

> Given a set of reference system samples $\{s_1, \ldots, s_l\}$, *model calibration* is the task of adjusting the values of the parameters, $\left(p_1^M, \ldots, p_n^M\right)$, so that

$$\begin{gathered} \left| y_{j,i}^S - \omega_j\left(\psi\left(x_{1,i}^S, \ldots, x_{q,i}^S\right), p_1^M, \ldots, p_n^M\right) \right| \le \varepsilon_j; \\ \forall j \in \{1, \ldots, k\}, \quad \forall i \in \{1, \ldots, l\} \\ \Leftrightarrow \\ \left| y_{j,i}^S - \hat{y}_{j,i}^S \right| \le \varepsilon_j \; ; \forall j \in \{1, \ldots, k\}, \quad \forall i \in \{1, \ldots, l\} \end{gathered} \tag{1}$$

Where *j* is the index of the response variable and *i* is the index for the flow regime or reference sample. Hence *k* is the number of response variables and *l* is the number of flow regimes. The introduction of tolerance deviations between reference system outputs and model outcome in Eq. (1) opens up the opportunity to utilize it in a calibration optimization formulation. The process of parameter adjustment can then be handled by an optimization algorithm instead of e.g. manual ad hoc adjustment.

According to the definition above the parameter values can be evaluated in relation to the *i*^th^ reference system sample. In this work different reference systems correspond to different flow regimes depending on the chosen reference system parameters (aperture width, hopper angle, sliding plane angle). The possible configurations of different hopper aperture, angle and plane angle are illustrated in Figure 8.

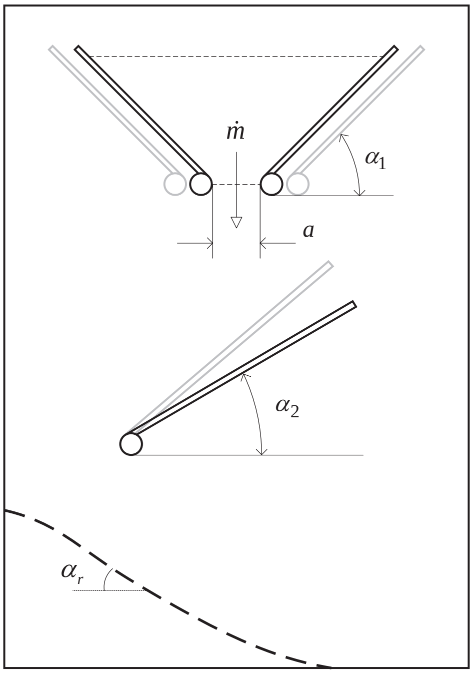

Figure 8. Calibration device configuration and adjustments made to arrive at different flow regimes.

The hopper angle, aperture and the angle of the sliding plane influences the particle flow behaviour hence the hopper mass flow and the repose angle of the settled bed.

Optimization Formulation

The calibration can now be formulated as a multi-objective optimization (MOO) problem according to Eq. (2). Each reference system configuration generates a corresponding tolerance deviation error and two response variables are evaluated. The optimization problem can be written on negative null form according to Papalambros (Papalambros, 2000).

$$\min_{\mathbf{x}} \; F(\mathbf{x}) = \left[f_1(\mathbf{x}), \ldots, f_j(\mathbf{x}), \ldots, f_n(\mathbf{x}) \right]$$

where,

$$f_j(\mathbf{x}) = \sum_{i=1}^{k} \frac{\left| \overline{y}_{i,j,exp}(\mathbf{x}) - \hat{y}_{i,j,sim}(\mathbf{x}) \right|}{N_j} \tag{2}$$

$$s.t. \begin{cases} g(\mathbf{x}) \le 0 \\ h(\mathbf{x}) = 0 \\ \mathbf{x} \in \left]0,1\right[\end{cases}$$

The approach of using weighted sum of squares has been used before by Kruggel-Emden (Kruggel-Emden et al., 2007). For more theoretical background on optimization the reader is referred to e.g. Papalambros (Papalambros, 2000) or Belegundu (Belegundu, 1999).

CONCLUSION

Calibration of DEM models needs to be performed on three levels according to the adopted V-model. On all levels the exercise of finding the correct model parameters may be handled as an optimization problem where the error is minimized using a multi-objective optimization formulation.

The definition of pragmatic congruence is a practical way of handling the problem of comparing the model and reference systems during the calibration.

ACKNOWLEDGEMENT

This work has been carried out within the Sustainable Production Initiative and the Production Area of Advance at Chalmers. The support is gratefully acknowledged.

The authors would also like to acknowledge the support from Ellen, Walter and Lennart Hesselmans foundation for scientific research and MinFo.

REFERENCES

Barrios, G.K.P., de Carvalho, R.M., Kwade, A., Tavares, L.M., Contact parameter estimation for DEM simulation of iron ore pellet handling. Powder Technology, 2013, **248(0)**, 84-93.

Belegundu, A.D., Chandrupatla, T.R., *Optimization Concepts and Applications in Engineering*. 2nd edn. 1999, Cambridge University Press.

Coetzee, C.J., Els, D.N.J., Calibration of discrete element parameters and the modelling of silo discharge and bucket filling. Computers and electronics in agriculture, 2009, **65**, 198-212.

Coetzee, C.J., Nel, R.G., Calibration of discrete element properties and the modelling of packed rock beds. Powder Technology, 2014, **264(0)**, 332-342.

Combarros, M., Feise, H.J., Zetzener, H., Kwade, A., Segregation of particulate solids: Experiments and DEM simulations. Particuology, 2014, **12(0)**, 25-32.

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

Frankowski, P., Morgeneyer, M., Calibration and validation of DEM rolling and sliding friction coefficients in angle of repose and shear measurements. AIP Conference Proceedings, 2013, **1542(1)**, 851-854.

González-Montellano, C., Ramírez, Á., Gallego, E., Ayuga, F., Validation and experimental calibration of 3D discrete element models for the simulation of the discharge flow in silos. Chemical Engineering Science, 2011, **66(21)**, 5116-5126.

Grima, A.P., Wypych, P.W., Development and validation of calibration methods for discrete element modelling. Granular Matter, 2011, **13**, 127-132.

Gröger, T., Katterfeld, A., 2006. On the Numerical Calibration of Discrete Element Models for the Simulation of Bulk Solids, In *16th European Symposium on Computer Aided Process Engineering*. Elsevier B.V.

Hanley, K.J., O'Sullivan, C., Oliveira, J.C., Cronin, K., Byrne, E.P., Application of Taguchi methods to DEM calibration of bonded agglomerates. Powder Technology, 2011, **210(3)**, 230-240.

Hofmann, M., On the Complexity of Parameter Calibration in Simulation Models. The Journal of Defense Modeling and Simulation, 2005, **2(4)**, 217-226.

Kruggel-Emden, H., Simsek, E., Rickelt, S., Wirtz, S., Scherer, V., Review and extension of normal force models for the Discrete Element Method. Powder Technology, 2007, **171(3)**, 157-173.

Papalambros, P.Y., Wilde, D.J., *Principles of Optimal Design: modelling and computation*. 2nd edn. 2000, Cambridge university press.

Schlesinger, S.e.a., Terminology for model credability. Simulation, 1979, **32(3)**, 103-104.

Wang, Y., Tonon, F., Modeling Lac du Bonnet granite using a discrete element model. International Journal of Rock Mechanics and Mining Sciences, 2009, **46(7)**, 1124-1135.

Yoon, J., Application of experimental design and optimization to PFC model calibration in uniaxial compression simulation. International Journal of Rock Mechanics and Mining Sciences, 2007, **44(6)**, 871-889.