CHEMICAL ENGINEERING TRANSACTIONS
VOL. 74, 2019
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it
Guest Editors: Sauro Pierucci, Jiří Jaromír Klemeš, Laura Piazza

ISBN 978-88-95608-71-6; **ISSN** 2283-9216
DOI: 10.3303/CET1974064

Calibration of DEM Simulation of Cohesive Particles

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DEM is a useful instrument to successfully design, optimise or simply analyse systems and equipment for granular materials in many applications where interparticle forces play a key role. In this paper, a study on the calibration of the parameters for the description of interparticle forces in DEM model is presented. Two different models for the interparticle forces have been used: a Hertz-Mindlin with Johnson-Kendall-Roberts (JKR) cohesive model and a Hertz-Mindlin with Linear cohesion model. By changing the model parameter and the time step, the simulations allow to evaluate the adhesion force between two particles. The calibrated value of the parameter can be chosen by a comparison between the force estimated, that is evaluated by means of the Rumpf-Molerus equation and that dependent on the Hamaker constant, with the simulation. However, it seems that both models are not suitable if a low time step is used. In fact, a small change of the model parameter could lead to a completely wrong estimation of the interparticle force.

1. Introduction

Discrete element method (DEM) is a computational method by which granular flow at an individual particle level is analyzed. DEM is used in many fields, such as mining, agriculture, geotechnical, mixing and milling applications, in order to design, study and optimise equipments or handle systems for loose granular materials. (Coetzee, 2017). All these applications can include interparticle cohesive forces (Obermayr et al., 2014), which can be caused by: the formation of liquid bridges among the particles (Xu et al., 2017), van der Waals and electrostatic forces (Chirone et al., 2018). In order to properly model cohesive materials, it is necessary to use a contact model which can capture the effect of cohesion on the mechanical behavior of the material. Different modelling approaches and DEM contact models have been proposed in literature to reproduce the cohesive forces. Some examples of these contact models are: the DEM mechanical model of cohesive soil with parallel bonds between particles (Zhang and Li, 2006), the Cohesive Discrete Element Method (Gröger et al., 2003). The main limit of these models is the computational time because it is necessary to reproduce in the simulations particles with the same size of the actual ones. An alternative approach is to use larger particles and DEM contact models, which can capture the macroscopic cohesive behaviour of the powder (Obermayr et al., 2014).
For the correct application of DEM, the model calibration is a crucial process. Calibration is the process to determine a set of DEM input parameters by comparing the powder bulk behaviour from physical experiments with the results of the simulations (Salehi et al., 2018). To start a DEM simulation, a contact model has to be implemented with the corresponding input parameters. A contact model describes how elements behave when they come into contact with each other. Among the most used contact models are: the Hertz-Mindlin (no slip), the Hertz Mindlin with JKR (Johnson-Kendall-Roberts) cohesive model (Baran et al., 2009), the Linear Cohesion (Romaní Fernández and Nirschl, 2013). The Hertz-Mindlin (no slip) is the default model used in EDEM due to its accurate and efficient force calculation. It accounts for the effects of contact of two elastic spheres. In this model: the normal force component is based on Hertzian contact theory (Hertz, 1881), the tangential force model is based on Mindlin-Deresiewicz work (Mindlin, 1989; Mindlin and Deresiewicz, 1989). Hertz-Mindlin with JKR cohesive model is a cohesion contact model that accounts also for the influence of van der Waals forces within the contact zone and allows the user to model strongly adhesive systems, e.g. dry powders or wet materials. The Linear Cohesion model modifies a certain base contact model (e.g. the Hertz Mindlin) by adding a normal cohesion force. The three models are implemented in EDEM by DEM Solutions

Paper Received: 18 April 2018; Revised: 8 September 2018; Accepted: 11 December 2018

Please cite this article as: Lupo M., Sofia D., Barletta D., Poletto M., 2019, Calibration of Dem Simulation of Cohesive Particles, Chemical Engineering Transactions, 74, 379-384 DOI:10.3303/CET1974064

Ltd. Description of the models is reported in the Edem 2019 documentation. This paper aims at finding the effect of the time step length on the values of the contact force in the calibration process of the model.

2. Materials and methods

2.1 Experimental

Glass beads, whose properties are reported in Table 1, have been used to evaluate the contact force.

Table 1 Material properties and interparticle force: d_{sv} is the Sauter mean particle diameter; $d_{4,3}$ is the volume mean particle diameter; ϱ_b is the bulk density ; C is the cohesion; ϕ is the angle of internal friction; $F_{vdW,1}$ is the van der Waals force estimated from the powder flow properties according the Rumpf-Molerus equation (Chirone et al., 2016)*; A is the Hamaker constant, z_0 is the separation distance and $F_{vdW,2}$ is the adhesion force in terms of the Hamaker constant*

Material	d_{sv} (μm)	$d_{4,3}$ (μm)	ϱ_b (kg m^{-3})	C (Pa)	ϕ (°)	$F_{vdW,1}$ (10^{-6} N)	A (10^{-20} J)	z_0 (10^{-10} m)	$F_{vdW,2}$ (10^{-6} N)
Soda Lime Glass Beads	125	129	2500	75	25	1.07	6.5	2	6.77

A Schulze ring shear tester RST-01.01, equipped with a S-cell (internal volume of the cell of 203.58 cm^3; external and internal annulus diameter of the lid of 118 and 62 mm, respectively) has been used to infer the interparticle force. Standard procedure recommended for the ring shear tester RST-01.01, and the ASTM-standard (ASTM D6773, 2002) have been followed. Tests at consolidation stresses between 0.4 and 0.7 kg have been run and 4-5 shear points have been registered to obtain the corresponding yield locus. To acquire, visualize, and record the main data, measured during the shear experiments, a software application, developed in the LabVIEW environment (National Instruments), has been used. Additionally, the RSV 95 software version 2.1.0.1 for the RST-01.01 Schulze shear tester has been used to derive the yield loci, the flow function and the other relevant flow properties of the powder. Following the procedure adopted by Tomasetta et al. (Tomasetta et al., 2014), for each consolidation condition, the tensile strength, σ_t, can be calculated as follows:

$$\sigma_t = \frac{C}{tan\,\phi} \tag{1}$$

where σ_t is the tensile strength, C is the cohesion and ϕ is the angle of internal friction. The Van der Waals force is related to σ_t in the following way:

$$F_{vdW,1} = \sigma_t\, d_{sv}^2\, \frac{\varepsilon}{1-\varepsilon} \tag{2}$$

where d_{sv} is the particle Sauter mean diameter and ε is the porosity of the bulk solid. Equation (2) follows the the Rumpf (Rumpf, 1970) and Molerus (Molerus, 1975) approach and relates the tensile strength to the binary interparticle forces. Equations (1) and (2) can be used to have an estimate of the interparticle force from measured powder flow properties. Another way to make a theoretical estimation of the van der Waals force is the following:

$$F_{vdW,2} = \frac{A\,r}{12\,z_0^2} \tag{3}$$

where A is the Hamaker constant, r is the mean curvature radius at the contact point and z_0 is the separation distance. (Israelachvili, 2011)

2.2 Modeling

In DEM simulation, two different models have been tried: Hertz-Mindlin with JKR cohesive model and Hertz-Mindlin with Linear cohesion model. According to the Johnson-Kendall-Roberts theory (Johnson et al., 1971), the normal elastic contact force depends on the overlap δ and the interaction parameter, i.e. the Surface Energy γ in the following way:

$$F_{JKR} = -4\sqrt{\pi\gamma E^*}\, a^{3/2} + \frac{4\,E^*}{3\,R^*}\, a^3 \tag{4}$$

$$\delta = \frac{a^2}{R^*} - \sqrt{\frac{4\pi\gamma a}{E^*}} \tag{5}$$

where: a is the contact radius, while E^* and R^* are the equivalent Young's Modulus and the equivalent radius, respectively, and are defined as:

$$\frac{1}{E^*} = \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j} \tag{6}$$

$$\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j} \tag{7}$$

where E_i, ν_i , R_i, and E_j, ν_j, R_j, are the Young's Modulus, the Poisson ratio and the radius of each sphere in contact, respectively. For $\gamma = 0$, F_{JKR} turns into Hertz-Mindlin normal force. The maximum value of the cohesion force occurs when particles loose the physical contact. This value is called pull-out force, and it is given by:

$$F_{pullout} = -\frac{3}{2}\pi\gamma R^* \tag{8}$$

Therefore, the maximum cohesion force depends on the radius of the particles and on the Surface Energy γ.
In the case of Hertz-Mindlin with the Linear Cohesion, the normal cohesion force takes the form:

$$F_{cohesion} = k\,A \tag{9}$$

where A is calculated as

$$A = \pi \times (2 \times R \times normal\ overlap) \tag{10}$$

and R is the radius of the particle considered; the normal overlap is the overlap between two spheres; and k is a Cohesion Energy Density with units J m^{-3}. In this case, the interparticle force depends on the radius of the particles, the overlap and on the cohesion Energy Density. In the following surface energy and energy density will be considered as parameters to be fitted on possible experimental values of interparticle forces measured on real powders with non-spherical particles and, therefore, they are not necessarily related to values of surface energy and energy density with a strict physical meaning.

2.3 Simulation

To find the model that best allows to determine the actual interparticle force, i.e. the van der Waals force, a specific simulation procedure has been developed by means of the EDEM software. The simulation consists in the following steps (Figure 1): a) generation of two single particles: one particle on a plane and the other one on another plane. Both the planes have a central hole to block the particle in a defined position. Moreover, the planes are exactly one on the other; b) downward movement of the upper plane on the lower one, at a distance such that the upper particle just touches the other particle; c) Upward movement of the upper plane to a defined height.

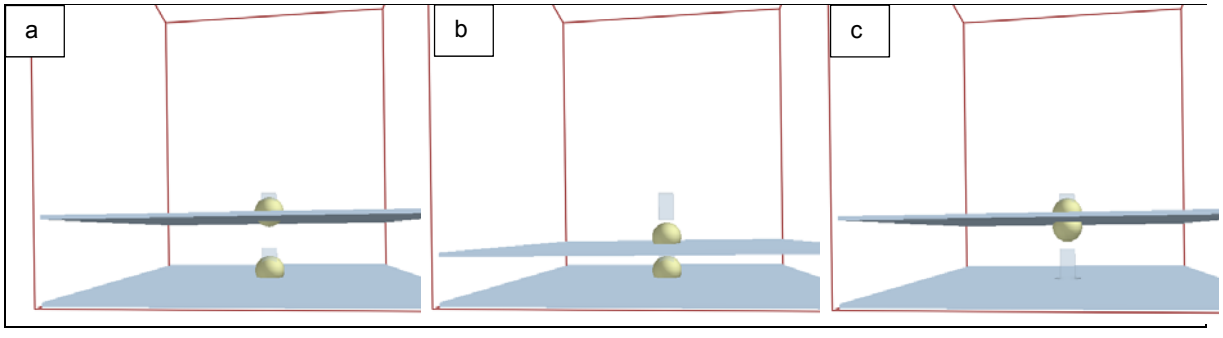

Figure 1 Different steps in the EDEM simulation to evaluate the interparticle force

A number of simulations have been carried out with EDEM with both the models. The bulk and the equipment material properties used are those reported in Table 2. In the first case, in which the Hertz-Mindlin with JKR cohesive model was considered, in the different simulations two parameters have been changed: the time

step and the Surface Energy. In particular, the Surface Energy, was changed between 0 and 500 J m^{-2}. In the second case, in which the Hertz-Mindlin model with Linear cohesion was assumed, the time step and the cohesion Energy Density have been changed. The interparticle force has been evaluated as the constant value of the maximum normal contact force between the particles, once the upper plane has reached a certain distance with respect to the lower plane and the lower particle is consequently attracted from the other one without being compressed. Hence it is assumed that the evaluated force corresponds only to the attractive component of the resulting force acting between the particles.
The time step was considered as a model parameter. It is the increment of time between calculative iterations. The time step is generally chosen as a fraction of the critical Rayleigh time step, that is the natural oscillation period of the mass-spring system made by the particle and the elastic contact (Marigo and Stitt, 2015):

$$\Delta t_c = \frac{\pi R \sqrt{\varrho_p / G}}{0.1631\nu + 0.8766} \tag{11}$$

where ϱ_p is the particle density, G is the material shear modulus at the contact. The normal range for the time step is between 10 % and 40 % of the critical Raleigh time step, as reported in the Edem 2019 documentation. The higher the particle energy in the simulation (higher forces, faster collisions) the lower should be the time step value. A time step equal to 20 % of the Raleigh time step is the default value recommended for EDEM codes. The smaller the time step, the more data points are produced. A large number of data points produce results with a very fine level of detail; however, the simulation time will be longer due to the increased number of calculations required. If the time step is too large, particles can behave erratically.

3. Results and discussion

From the tests with the Schulze ring shear tester at different normal forces, an average value for the cohesion and for the angle of internal friction has been measured. The values are reported in Table 1, together with the corresponding value of the van der Waals force, according to Eq. (2) and Eq. (3). The values used of A and z_0 have been taken from Israelachvili (Israelachvili, 2011). Given the elastic nature of the glass beads, the van der Waals force, calculated with Eq. (2), resulted to be scarcely dependent on the consolidation level.

Table 2 Particle and wall properties in the EDEM simulation: d_p is the particle diameter, ν is the Poisson's Ratio; ϱ_p is the particle density; G is the Shear Modulus

Material	d_p (10^{-6} m)	ν	ϱ_p (kg m^{-3})	G (10^7Pa)	Restitution coeff.	Static Friction	Rolling Friction
Glass beads	100	0.25	2500	1	0.5	0.45	0.15
Steel (wall material)	-	0.25	4000	1000	0.5	0.45	0.15

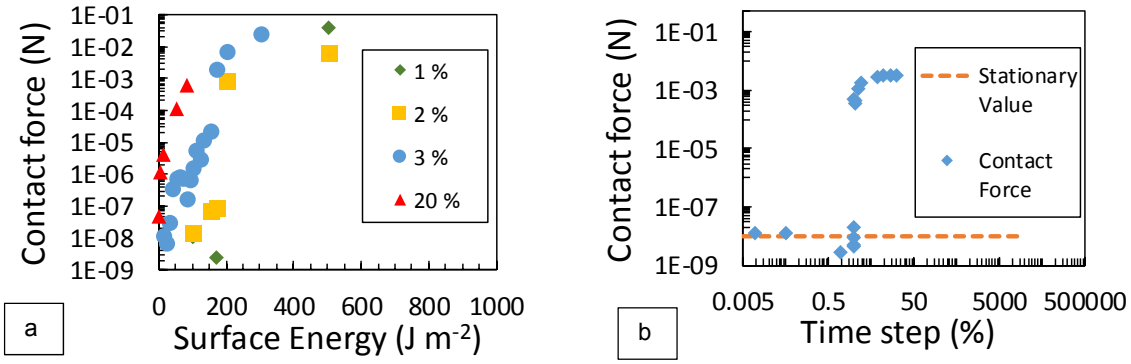

Figure 2 a) Evaluation of the interparticle force for different Surface Energies and at different time steps, evaluated as a fraction of the Raleigh time step; b) Search for the minimum required time step (fraction of the Raleigh time) which ensures the same interparticle force at the same Surface Energy, that in the analysis is 170 J m^{-2}. The two graphs have been obtained by using the Hertz-Mindlin interparticle contact force with the JKR cohesive model

3.1 Hertz-Mindlin with JKR cohesive model

Figure 2 represents the results of the simulated contact force at different surface energies (Figure 2a) and different time steps (Figure 2b) using the Hertz-Mindlin with JKR cohesive model. Inspection of the figure indicates that, in general, the lower the time step, the lower the contact force, for the same Surface Energy (Figure 2a).

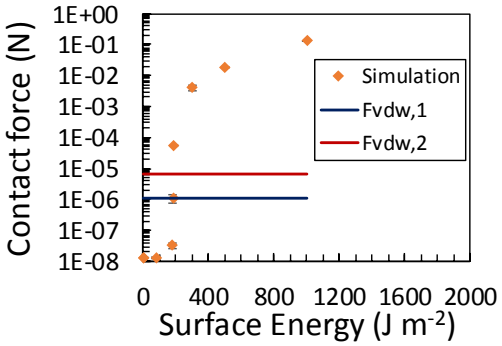

Figure 3 Evaluation of the interparticle force (♦) at different Surface Energies for a time step of the 2 % of the Raleigh time, and comparison with the expected value, expressed by $\boldsymbol{F}_{vdW,1}$ and $\boldsymbol{F}_{vdW,2}$. The model used is the Hertz-Mindlin with JKR cohesive model

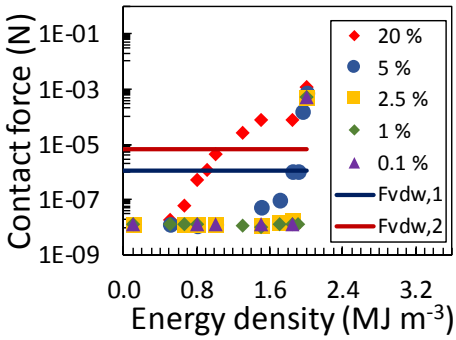

Figure 4 Evaluation of the interparticle force at different time steps, evaluated as a percentage of the Raleigh time step, and at different Energy Densities, and comparison with the expected value, expressed by $\boldsymbol{F}_{vdW,1}$ and $\boldsymbol{F}_{vdW,2}$. The model used is the Hertz-Mindlin with Linear cohesion

It appears that for a time step between 1 and 2 %, the trends are close and similar. As above mentioned, the lower the time step, the more accurate is the force evaluation. Therefore, it is necessary to understand which time step is the best to be chosen. In order to find this time step, simulations for the same value of the Surface Energy, i.e. 170 J m^{-2}, and at different time steps have been carried out (Figure 2b). From the results, it follows that a time step up to 2 % of the critical time step is able to provide almost the same value of the force, which is represented in the figure with the orange hyphenated line. Therefore, a time step equal to 2 % of the critical time step can be considered as the best tradeoff between calculation time and accuracy of results. Hence with a time step of 2 %, simulations at different surface energies have been performed (Figure 3). Simulation includes some stochastic elements due to the particle generation process. Therefore, results may change between simulations made with the same parameters. Therefore, each simulation was repeated three times to verify the correctness of the evaluated cohesive force. With a time step of 2 %, simulations lasted approximately 20 minutes. Error bars have been calculated on the basis of the standard deviation between force results. It appears that simulations are reproducible. In fact, error bars are very short and not clearly visible in the graph. Inspection of Figure 3 shows a steep change in the contact force by changing the Surface Energy around 200 J m^{-2}. This finding suggests that, for the particles under examination, and with the low value of the time step, required to have stable results of the contact force, small variations of the Surface Energy can bring to order of value changes of the interparticle forces. Unfortunately, the desired values of the contact forces, represented by the red and blue lines (referring to the experimentally estimated and to the theoretical values) are fully contained within this wide range of change of the modelled contact force. Therefore, adoption of the Hertz-Mindlin with JKR cohesive model for the contact forces, makes it difficult to choose a proper value of the Surface Energy parameter without avoiding errors in the interparticle force evaluation.

3.2 Hertz-Mindlin with Linear cohesion model

Figure 4 reports results of the calculated interparticle force using the Hertz-Mindlin with Linear cohesion model. Different simulations have been carried out, by changing the Energy Density and the time step. Also in this case, the force is highly dependent on the time step, although for a time step less than or equal to 2.5 %, the calculated force does not change for similar values of the Energy Density. In addition, still similarly to the previous case, the expected desired force (blue and red lines) is obtained in correspondence of the portion of the curve in which a small variation in the Energy Density can lead to large changes of the calculated force. Simulations with a time step of 2.5 % lasted between 15 and 20 minutes.

4. Conclusions

Two different models for the evaluation of the interparticle forces have been used to calibrate the model parameters: Hertz-Mindlin with JKR cohesive model and Hertz-Mindlin with Linear cohesion. The calibrated value of the parameter has been chosen by a comparison between the force estimated with the simulation. Even if a time step between 10 and 40 % of the critical Raleigh time step is usually suggested, in this work lower optimal percentages have been found out: 2 % and 2.5 %, for Hertz-Mindlin with JKR cohesive model

and Hertz-Mindlin with Linear cohesion, respectively. In the case of particles with an average diameter of 100 μm, it seems that both the Hertz-Mindlin with JKR cohesive model and the the Hertz-Mindlin with Linear cohesion model, which can be implemented in the EDEM code, are not suitable if a low time step is used. In fact, in both cases a small change of the model parameter used could lead to a completely wrong estimation of the interparticle force. A possibility could be that of choose a higher time step, e.g. 20 %, and a value of the model parameters, the Surface Energy and the Energy Density respectively, for which the expected force can be obtained. In the future it might be possible to choose different cohesive models, which are implemented in the EDEM software, such as: Edinburgh Elasto-Plastic Adhesion Model, Hertz-Mindlin with JKR Version 2 and Hysteretic Spring. Furthermore, other materials than glass beads could be experimentally analyzed and studied with the use of statistics to evaluate which of the parameters are most significant for each model.

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