A novel approach to particle characterization for discrete element method by means of artificial neural networks

L. Benvenuti[a,*], S. Pirker[a], C. Kloss[b]

[a] *JKU Department of Particulate Flow Modelling - Linz*
[b] *DCS Computing - Linz*

Abstract

Discrete Element Method (DEM) simulations are widely used to model and understand particle behavior. It is important to note that each combination of DEM-micro parameters gets different bulk-macro behavior. As a consequence, a straight-forward trial-and-error calibration procedure is prohibitively computationally expensive to fathom the micro-macro transition relationship. A limited number of combinations have been simulated, through 2000 shear cell numeric test and 300 $static-angle-of-repose$ ($SAOR$) numeric test. The DEM parameters of the simulations have been used as inputs of feed forward Multilayer Perceptron Neural Networks ($MLPNN$), while the bulk values and behavior as targets for the Neural Networks (NN). A backpropagation reinforcement learning training algorithm has been used (scaled conjugate gradient). A NN has been created for each bulk parameter investigated. 15% of the simulations have been excluded from the training processes. They have been used to define per each NN the correct number of neurons in the hidden layer, based on an R^2 maximization. Then each trained NN received as input one million different combinations. The bulk solids were characterized using shear cell testers. The DEM coefficients were obtained by fitting NN outputs to experimental data (within a 5% error). Further, we validated the DEM parameters by means of $SAOR$ experiments and $SAOR$ simulations-trained NN. The validation agreement was also within reliable limits (5% error). The calculated DEM coefficients of iron ore, limestone and silibeads accord well with published data and in-house experiments.

Keywords: Meshless methods (DEM), Rheology, experimental validation studies, process industries, process metallurgy, LIGGGHTS, Material characterization, Artificial Neural Networks

1. Introduction

Particles in various forms - ranging from raw materials to food grains and pharmaceutical powders - play a major role in a variety of industries, including process industry and metallurgy. In his book, Holdich [5] stated that "between 1 and 10% of all the energy is used in comminution, i.e. the processes of crushing, grinding, milling, micronising". However, a univocal method to characterize these particles has so far not been established. From the experimental point of view, the main issues are the difficult setups and the general reliability and reproducibility of the tests. From the numerical point of view, no general procedure is available, and the existence of a mathematically unique solution describing macro/micro particle contact has yet to be proved. Moreover, in a recent study, Krantz et al. [7] implied "that the dynamic properties of a powder cannot be applied to universally predict the static properties of a powder, and, likewise, the static properties cannot be used to predict dynamic properties".

Discrete Element Method (DEM) simulations are widely used to understand particle behavior. Mishra and Rajamani [8] defined the DEM as "a special class of numerical schemes for simulating the behavior of discrete, interacting bodies". The force that particle i exerts on particle j is defined as:

$$m\ddot{x}_{ij} + c\dot{x}_{ij} + kx_{ij} = F_i. \quad (1)$$

Further details on the method can be found in Poschel and Schwager [10]. $LIGGGHTS$ (LAMMPS improved for general granular and granular heat transfer simulations) is one of the most powerful open source DEM simulation software packages available. The models it can analyze are described in detail in the literature, see

*Corresponding author
Email address: luca.benvenuti@jku.at (L. Benvenuti)

Kloss et al. [6]. In combination with shear cell tester simulation developed by Aigner et al. [1], *LIGGGHTS* has correctly defined the coefficient of sliding friction for coarse round particles - a critical parameter describing inter-particle friction in medium to dense granular flows simulations.

Since the bulk solid is represented by perfect spheres, the only parameter the software uses to describe its shape is the radius of the particle (R). However, since the shape is one of the most relevant aspects defining particle behavior, we consider the coefficient of rolling friction (μ_r) as an additional DEM shape parameter. It is proportional to the torque counteracting the rotation of the particle and defined as (Eq. 9):

$$\mu_r = \tan(\iota). \tag{2}$$

The last $DEM - micro$ parameter investigated is the $coefficient - of - restitution$ (COR), given its centrality in the whole model. DEM simulations have recently been used to reduce the bias of the experiments, and more precise devices such as the Schulze ring shear cell tester (SRSCT)(see Schulze et al. [11]) have been built. A dedicated workflow that combines experiments and simulations must now be devised following the Design of Experiments method, as illustrated by Grossman and Vecchio [3].

The main goal of this new procedure should be the characterization of non-spherical particles, especially the DEM coefficients of friction and restitution, following standardizable steps. With this objective in mind, we profited from the shear cell experimental and numerical setup in combination with $LIGGGHTS$ simulation to improve the accuracy and the range of applicability of particle characterization. Nevertheless, DEM simulations require tens of thousand of particles to achieve the necessary reliability for a straight-forward trial-and-error calibration procedure. The calibration compels to identify the $DEM - micro$ combination of parameters that numerically grants the same $bulk - macro$ behavior experimentally registered, measured as $steady - state - flow/pre - shear\ coefficient - of - internal - friction$ (μ_{ie-ps}), $incipient - flow/shear\ coefficient - of - internal - friction$ (μ_{ie-s}) and $bulk\ density$ (ρ_b). Furthermore, we used Hertz' Law for the particle-particle and particle-wall interactions. Its complexity increased the computational effort to fathom the micro-macro transition relationship. Thus, the time necessary to perform all the possible $DEM - micro$ parameters combinations became boundless. In order to overcome this doomed situation we decided to operate artificial neural networks, as suggested by Antony et al. [2]. A limited number of combinations have been simulated, designed to maxime the representativity. Following the indications of Vaferi et al. [12], *feed forward Multilayer Perceptron Neural Networks (MLPNN)* have been handled. Their trustworthiness, together with a backpropagation reinforcement learning training algorithm(scaled conjugate gradient), has been widely demonstrated in the literature, see Haykin [4]. The DEM parameters of the simulations have been used as inputs of the Neural Networks (NN), while the bulk values and behavior as targets for them. Furthermore, the best practice suggested by Vaferi et al. [12] demands to establish the most appropriate number of neurons inside the hidden layer of each NN. As in literature, this goal has been achieved by first excluding 15% of the simulations from the training processes. We then fed the NN with the same $DEM - micro$ parameters of these simulations. Subsequently, we controlled the square regression error between the $bulk - macro$ behavior in these simulations and in the output of the NN. Finally, we selected for each $bulk - macro$ behavior property (μ_{ie-ps}, μ_{ie-s} and ρ_b) the NN with the number of neurons that provided the maximum R^2. Later, each of these three trained NN received as insertion $1M$ different combinations $DEM-micro$ parameters. We then compared their outputs against the values provided by the shear cell experiments (within a 5% error), gaining the $DEM-micro$ coefficients range. Oberkampf and Roy [9] prescribes an ulterior validation step. To accomplish his demand, we realized a $static - angle - of - repose$ ($SAOR$) experiment and $SAOR$ simulation. Furthermore, we performed the $SAOR$ simulation, again with the same limited number of combinations. These allowed to determine two $bulk - macro$ behavior properties, the $angle - of - repose$ (AOR) and the $bulk\ density$ (ρ_b). Likewise, we then trained NN and optimized the number of their neurons. Later, each of these two trained NN received as insertion the $DEM - micro$ coefficients range previously determined. We then compared their outputs against the values provided by the $SAOR$ experiment (again within a 5% error), gaining a narrower $DEM - micro$ coefficients range. Since this study was supported by the metallurgical industry, the materials examined were: silibeads (2 mm), coke, iron ore, limestone (all 0-3.15 mm). For the same reason, cohesive materials have been excluded from this study.

trotaculo

2. Method

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam

arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

$$e = mc^2 \tag{3}$$

2.1. Discrete element method

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

$$F_{ij} = \begin{cases} F_{n,ij} + F_{t,ij} = \left(k_n \delta_{n,ij} + \gamma_n v_{n,ij}\right) + \left(k_t \delta_{t,ij} + \gamma_t v_{t,ij}\right) \\ 0 \end{cases} \tag{4}$$

2.2. Artificial Neural Networks

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

$$\begin{aligned} M_r &= M_r^k, \\ M_{r,ti+\Delta ti}^k &= M_{r,ti}^k - k_r \Delta \theta_r, \\ |M_{r,ti+\Delta ti}^k| &\le M_r^m = \mu_r R_{eq} F_n. \end{aligned} \tag{5}$$

2.3. Experimental setup

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

$$\begin{aligned} \frac{1}{E_{eq}} &= \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j}, \\ \frac{1}{G_{eq}} &= \frac{2(2+\nu_i)(1-\nu_i)}{E_i} + \frac{2(2+\nu_j)(1-\nu_j)}{E_j}, \\ \text{if } r < d, \frac{1}{R_{eq}} &= \frac{1}{R_i} + \frac{1}{R_j}, \\ \text{if } r > d, \frac{1}{m_{eq}} &= \frac{1}{m_i} + \frac{1}{m_j}, \\ \beta &= \frac{\ln(e)}{\sqrt{ln^2(e) + \pi^2}}, \\ S_n &= 2E_{eq}\sqrt{R_{eq}\delta_n}, \\ S_t &= 8G_{eq}\sqrt{R_{eq}\delta_n}, \\ k_r &= k_t R_{eq}^2. \end{aligned} \tag{6}$$

3. Results and discussion

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam

arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

$$F_{t,ij} \leq \mu_s F_{n,ij}. \tag{7}$$

3.1. DEM Simulations

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

$$\begin{aligned} k_n &= \frac{4}{3} E_{eq} \sqrt{R_{eq} \delta_n}, \\ \gamma_n &= 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_n m_{eq}}, \\ k_t &= 8 G_{eq} \sqrt{R_{eq} \delta_n}, \\ \gamma_t &= 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_t m_{eq}}. \end{aligned} \tag{8}$$

3.2. ANN model development

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

$$\mu_r = \tan(\iota). \tag{9}$$

3.3. ANN identification

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

$$m\ddot{x}_{ij} + c\dot{x}_{ij} + kx_{ij} = F_i. \tag{10}$$

3.4. ANN application

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

$$\begin{aligned} \phi_{e-psh} &= \arctan\left(\frac{\tau_{psh}}{\sigma_{n,psh}}\right), \\ \mu_{psh} &= \tan(\phi_{e-psh}). \end{aligned} \tag{11}$$

$$\phi_{e-sh} = \arctan\left(\frac{\tau_{sh}}{\sigma_{n,sh}}\right), \qquad (12)$$
$$\mu_{sh} = \tan(\phi_{e-sh}).$$

$$SC = \sum_{k=1}^{4}\sum_{l=1}^{4} C_{kl}. \qquad (13)$$

4. Conclusions

We have discussed the determination of DEM inter-particle friction and restitution parameters that are critical in medium to dense granular flow simulation. In particular, we have characterized the materials more commonly used in steel-making, with special regard to their non-sphericity and contact properties. We used a $SRSCT$, a $JSCT$ and an AOR tester to acquire experimental data. Then we employed a numerical shear cell tester and a numerical AOR tester for the simulations. We extended our numerical results by mean of artificial neural networks. Since our results for iron ore, limestone and glass silibeads are in very good agreement with published data and in-house experiments, we can conclude that the described experimental and simulation setup successfully defined the DEM parameters for these materials. Furthermore, the effectiveness of $LIGGGHTS$ as simulation software has again been demonstrated.

5. References