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

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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 angle of repose 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 Network (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 static angle-of-repose experiments and AOR 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

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Holdich [1]

$$C_{kl} = \begin{cases} 1 & \text{if } (|1 - \frac{\mu_{psh,sim}}{\mu_{psh,exp}}| < 5\% \text{ and } |1 - \frac{\mu_{sh,sim}}{\mu_{sh,exp}}| < 5\%), \\ 0 & \text{else.} \end{cases} \quad (1)$$

Krantz, Zhang, and Zhu [2]

2. Method

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

2.1. Discrete element method

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$$F_{ij} = \begin{cases} F_{n,ij} + F_{t,ij} = \left(k_n \delta_{n,ij} + \gamma_n v_{n,ij}\right) + \left(k_t \delta_{t,ij} + \gamma_t v_{t,ij}\right) & \text{if } r < d, \\ 0 & \text{if } r > d, \end{cases} \tag{3}$$

2.2. Artificial Neural Networks

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$$\begin{aligned} M_r &= M_r^k, \\ M^k_{r,ti+\Delta ti} &= M^k_{r,ti} - k_r \Delta\theta_r, \\ |M^k_{r,ti+\Delta ti}| &\le M_r^m = \mu_r R_{eq} F_n. \end{aligned} \tag{4}$$

2.3. Experimental setup

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$$\begin{aligned} \frac{1}{E_{eq}} &= \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j}, \\ \frac{1}{G_{eq}} &= \frac{2(2+\nu_i)(1-\nu_i)}{E_i} + \frac{2(2+\nu_j)(1-\nu_j)}{E_j}, \\ \frac{1}{R_{eq}} &= \frac{1}{R_i} + \frac{1}{R_j}, \\ \frac{1}{m_{eq}} &= \frac{1}{m_i} + \frac{1}{m_j}, \\ \beta &= \frac{\ln(e)}{\sqrt{ln^2(e) + \pi^2}}, \\ S_n &= 2E_{eq}\sqrt{R_{eq}\delta_n}, \\ S_t &= 8G_{eq}\sqrt{R_{eq}\delta_n}, \\ k_r &= k_t R_{eq}^2. \end{aligned} \tag{5}$$

3. Results and discussion

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$$F_{t,ij} \leq \mu_s F_{n,ij}. \tag{6}$$

3.1. DEM Simulations

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$$\begin{aligned} k_n &= \frac{4}{3} E_{eq} \sqrt{R_{eq} \delta_n}, \\ \gamma_n &= 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_n m_{eq}}, \\ k_t &= 8 G_{eq} \sqrt{R_{eq}} \delta_n, \\ \gamma_t &= 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_t m_{eq}}. \end{aligned} \tag{7}$$

3.2. ANN model development

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$$\mu_r = \tan(\iota). \tag{8}$$

3.3. ANN identification

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$$m\ddot{x}_{ij} + c\dot{x}_{ij} + kx_{ij} = F_{ij}. \tag{9}$$

3.4. ANN application

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$$\begin{aligned} \phi_{e-psh} &= \arctan\left(\frac{\tau_{psh}}{\sigma_{n,psh}}\right), \\ \mu_{psh} &= \tan(\phi_{e-psh}). \end{aligned} \tag{10}$$

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

$$SC = \sum_{k=1}^{4} \sum_{l=1}^{4} C_{kl}. \tag{12}$$

4. Conclusions

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