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Simulation of vibrated bulk density of anode-grade coke particles using discrete element method

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ABSTRACT

Packing density is an important quality parameter of calcined cokes used in aluminum industry to produce carbon anodes. Vibrated bulk density (VBD) test is a well established method to measure the packing density of coke samples. In the present work, Discrete Element Method (DEM) is coupled with a three-dimensional imaging technique to investigate the possibility of using DEM to simulate the packing behavior of calcined cokes. As the method verified, effects of shape, friction coefficient, size and size distribution of the particles on the VBD of cokes are also investigated. DEM simulations, in accordance with the experiments, show that vibrated bulk density of coke samples decreases as the content of coarse particles in the mixture increases. Moreover, it is shown that friction coefficient has a negative effect on the VBD value and this effect is more pronounced for the samples with lower sphericity. High friction coefficient restricts the movement and rearrangements of the particles and thus vibrational forces cannot effectively rearrange the particles and fill the porosities. Lower sphericity of coke samples not only induces a higher initial porosity level in the samples but it also increases the chance of formation of locks and particle bridges which result in lower VBD. Results also show that sphericity and friction coefficient have a synergic effect on the VBD of coke so that, for the samples with lower average sphericity the rate of decrease in VBD is higher with increasing the friction coefficient.

1. Introduction

Calcined coke is an important raw material for production of consumable carbon anodes in aluminum industry. Anode is made by mixing coke and pitch to prepare anode paste, which is then compacted and baked. Physical and chemical properties of raw materials must be taken into account to determine the paste formulation, which in turn affects the quality of the baked anode. Due to the frequent changes of sources of raw materials, the processing parameters should be adjusted accordingly in order to keep the quality consistency of the baked anodes. The adjustment of process parameters requires understanding the effect of each raw material properties on the anode quality.

Modeling approaches could be useful to simulate the process and to determine the right process parameters for a given set of raw materials. Choosing an appropriate model, which depends on the nature of the paste and its constitutive laws, is however crucial to obtain reliable simulation data.

Green anode is made either by pressing or by vibro-compacting the anode paste, which consists of two principal phases; a binder matrix (pitch + fine) and coke aggregates. Bulk density of calcined coke is used as an important gage in determination of pitch demand in anode production process [1–3].

Several works have been published in the last two decades dealing with the effects of different parameters on packing density of granular media such as [4–7]. White and Walton [8] studied the effects of particle shape on packing density of different packing systems using both theoretical and experimental methods. H.J.H. Brouwers [9] investigated the particle size distribution and porosity fractions in randomely packed beds. He addressed the parameters of analytical expressions for determining void fraction in packing of unimodal and bimodal spheres. Effects of particle shape on angle of repose of heaps have also been reported in the literature [10].

Discrete Element Method, introduced for the first time by Cundall and Strack [11] in 1979, is now used to simulate the behavior of granular materials in industrial applications specially where the dynamics and flow of a particulate material are of interest. In DEM simulations, rigid discrete elements, which are spheres in 3D and discs in 2D models, are used to model the granular material. The contact law between the elements defines the mechanical behavior of the bulk material. Using DEM, El Shourbagy et al. [12] showed that the angle of repose of dry granular materials depends on the particles shape and Columb friction coefficient.

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This work aims at exploring the possibility of using DEM to simulate the packing behavior of coke particles through vibrated bulk density (VBD) test. As the model verified by the experiments, effects of friction coefficient and sphericity of coke particles on VBD value is also investigated. VBD test is routinely used to measure the packing density of calcined coke and is considered as one of the important anode-grade coke specifications. The simulation is performed using PFC3D software. A three-dimensional imaging technique is used to capture the real shape of coke particles. Effects of particles shape and friction coefficient on the VBD of coke samples are therefore investigated by means of DEM modeling with PFC3D.

2. The numerical model

2.1. Principles of DEM

A three dimensional DEM model is composed of a combination of discrete spheres and walls. At the beginning, the position of all elements and walls are known so that the active contacts are easily determined. Then, according to the mechanical behavior of the material an appropriate force-displacement law is applied to each contact and the contact forces are calculated. Law of motion, Newton's second law, is then used to update the position and velocity of each ball.

One common contact model, which is widely used in DEM simulations, is linear contact model. This model is simply defined by assigning normal and shear stiffness values to the contacting elements (see Fig. 1). Normal and shear stiffness values of a contact are expressed as;

$$K^n = \frac{K_A^n . K_B^n}{K_A^n + K_B^n}$$

$$K^s = \frac{K_A^s . K_B^s}{K_A^s + K_B^s}$$

whrere K^n and K^s stand for the normal and shear stiffness of the elements (A and B in Fig. 1).

Having the shear and normal stiffness, one can obtain the force propagating at the contact point, if the balls are overlapping. Contact forces can be calculated according to the extent of the overlap (for normal contact force) and tangent movement (for shear contact force);

$$F^n = K^n . U^n$$

$$F^s = -K^s . \delta U^s$$

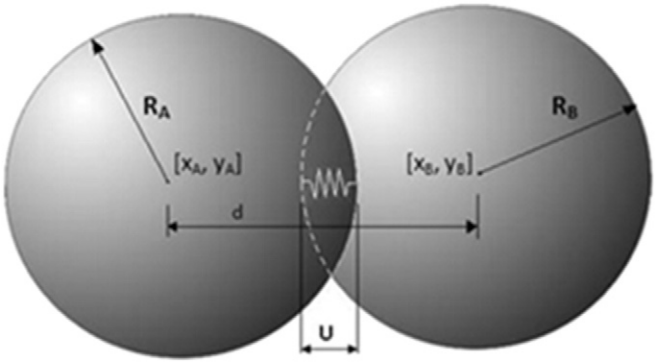

Fig. 1. Contact of two elements.

2.2. Movement of non-spherical particles

In PFC any kind of irregular shape particles can be generated as a clump composed of several touching or overlapping balls. Contact force calculations for balls within a clump is skipped during calculation cycle and only the contact force of a clump with neighboring clump/balls or walls are considered [13]. The basic mass properties of a clump are the total mass (m^{Cl}), center of mass (x_i^{Cl}), and moments and products of inertia (I_{ii} and I_{ij}). These properties can be mathematically expressed by the following equations [13];

$$m^{Cl} = \sum_{n=1}^{N_b} m^{[n]} \tag{1}$$

$$x_i^{Cl} = \frac{1}{m^{Cl}} \sum_{n=1}^{N_b} m^{[n]} x_i^{[n]} \tag{2}$$

$$I_{ii} = \sum_{n=1}^{N_b} \left\{ m^{[n]} \left(x_j^{[n]} - x_j^{Cl} \right) \left(x_j^{[n]} - x_j^{Cl} \right) + \frac{2}{5} m^{[n]} r^{[n]} r^{[n]} \right\} \tag{3}$$

$$I_{ij} = \sum_{n=1}^{N_b} \left\{ m^{[n]} \left(x_i^{[n]} - x_i^{Cl} \right) \left(x_j^{[n]} - x_j^{Cl} \right) \right\}; j \neq i \tag{4}$$

m^{Cl}, N_b are the mass of the clump and number of the balls in the clump, respectively. $x^{[n]}$, $r^{[n]}$, and $m^{[n]}$ are center of mass, radius and the mass of the n^{th} ball, respectively.

Moments and products of inertia are calculated with respect to a coordination system, which is attached to the center of mass of the clump and is aligned with the global axis system.

Translational motion of clumps is expressed as;

$$F_i = m \left(\frac{\partial^2 x_i}{\partial t^2} - g_i \right)$$

where F_i is the resultant force, m is the total mass of the clump, $\frac{\partial^2 x_i}{\partial t^2}$ is the acceleration vector and g_i is the gravity acceleration vector.

The resultant force, which is the sum of all externally applied forces acting on the clump, can be expressed as;

$$F_i = \widetilde{F}_i + \sum_{n=1}^{N_b} \left(\widetilde{F}_i^{[n]} + \sum_{c=1}^{N_c} F_i^{[n,c]} \right) \tag{5}$$

where $\widetilde{F}_i$ is the externally applied force on the clump, $\widetilde{F}_i^{[n]}$ is the externally applied force acting on ball (n), and $F_i^{[n,c]}$ is the force acting on ball (n) at contact (c).

The resultant moment about the center of mass of the clump is calculated by

$$M_i = \widetilde{M}_i + \sum_{n=1}^{N_b} \left(\widetilde{M}_i^{[n]} + \epsilon_{ijk} \left(x_j^{[n]} - x_j^{Cl} \right) F_k^{[n]} + \sum_{c=1}^{N_c} \epsilon_{ijk} \left(x_j^{[c]} - x_j^{[n]} \right) F_k^{[n,c]} \right) \tag{6}$$

in which $\widetilde{M}_i$ is the externally applied moment acting on the clump, $\widetilde{M}_i^{[n]}$ is the externally applied moment acting on ball (n), $F_k^{[n]}$ is the resultant force acting on the centroid of ball (n), and $F_k^{[n,c]}$ is the force acting on ball (n) at contact (c).

Rotational motion of a clump is given by the vector equation of $M_i = H_i$, where $\dot{H}_i$ is the time rate of change of the angular momentum of the clump. $\dot{H}_i$ can be written as

$$\dot{H}_i = \dot{\omega}_i I_{ii} - \dot{\omega}_j I_{ij} + \in_{ijk} \omega_j (\omega_k I_{kk} - \omega_l I_{kl}); (j \neq i, l \neq k) \tag{7}$$

where I is the moment of inertia, and ω and $\dot{\omega}$ are angular velocity and angular acceleration about the principal axes respectively.