Effects of Bulk Density and Inter-particle Contacts on Electrical Resistivity of Calcined Coke Mixes

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Abstract

Packing density of particles is an important factor for a variety of applications of granular materials. In the present work, a three dimensional imaging technique is coupled with the Discrete Element Method (DEM) to model anode grade calcined coke particles. Coke aggregate recipe of industrial pre-baked anodes is modeled with DEM and then the pore size distribution in this packing is numerically measured. Results of the measurements are used to propose a new aggregate recipe. The proposed recipe is examined by its electrical resistivity and packing density. Results show that the proposed recipe holds a better packing density and lower electrical resistivity. It is shown that the inter-particle contact density is lower in the new recipe which results in lower electrical resistivity.

Keywords: Calcined coke, Discrete Element Method, Packing density, Electrical resistivity

1. Introduction

Particle packing is an old problem [1] which exists in different applications and industries such as construction, pharmaceuticals, food processing and agriculture [2]. Determination of conditions leading to maximum packing density is still a challenging work when the particles have irregular shapes and a wide size distribution.

Electrical current transfer in granular media has also considerable importance in a variety of applications such as electronics, metallurgical processes, railway transportation and geology [3]. Packing density and electrical resistivity of particles both are of interest for aluminum production. Pre-baked carbon anodes for the aluminum smelting process are made with granulated calcined coke mixed with binder pitch. Coke particles make up around 65 wt. % of an anode and thus the physical, chemical and mechanical properties of the coke have a considerable impact of anode quality. Effects of coke particles' bulk density on the air permeability of the baked anodes [4] and shape of coke particles on the compaction behavior of green anode paste [5] have been already investigated. Homogeneity, high density, low air permeability and low electrical resistivity are important quality factors which anodes are expected to hold.

Industrial dry mix recipe of anode paste is given in Table 1. Coke particles make up the skeleton for the anode and pitch binds the particles together providing the integrity of the mixture. A part of the pitch is vaporized during the baking process causing pores and shrinkage cracks. Binder matrix (pitch + fine coke particles) is also the most reactive part of the anode block to air and CO_2 attacks [6,7]. Underpitched anodes, on the other hand, have low apparent density and poor mechanical properties [8]. Therefore, if the coke aggregate recipe can be modified to have higher amount of coarse particles without compromising the density, pitch demand for this recipe could be reduced, resulting in positive effects on final properties of anode.

The Discrete Element Method (DEM) has a proven capability [9-13] in investigating the packing behavior of irregular-shape particles. For example in [9] the authors have reported the performance of DEM simulations in predicting the vibrated bulk density of coke aggregates.
In 2015, the authors have used DEM with a technique called void tracking [13], to study and modify the industrial recipe for aggregates in anode paste.

In the present work, void tracking is engaged to study the dry aggregate recipe used in aluminum industry to make anodes and the modified recipe is investigated for its density and electrical resistivity. Then, DEM is used to understand the variations in electrical resistivity for different samples.

Table 1. Typical coke particle recipe, used as reference

Size range (US sieve No.)	Size range (mm)	Content (wt. %)
-4+8	2.36 - 4.75	33.6
-8+14	1.4 - 2.36	15.3
-14+30	0.600 - 1.4	17.7
-30+50	0.300 – 0.600	19.4
-50+100	0.150 – 0.300	13.9

2. The Numerical Model

In DEM complex behavior of material is simulated by assigning an appropriate force-displacement law to the contacts between the elements of the model. Newton’s law of motion is then applied to all the elements to determine the acceleration and thus the new position of the elements at the next time-step. This concept is shown in Figure 1.

Simple elastic contact is a common model in DEM simulations to define force-displacement behavior of elastic materials. This model is equivalent to mechanical springs in normal and shear directions. The stiffness of the springs is a consequence of the material’s properties and is related to the elastic modulus. Details of this model can be found in [14].

Coke particles have irregular shapes but the basic elements of DEM are spheres in 3D. Thus, rigid clusters of overlapping spheres are used to model the real shape of coke aggregates. Sliding motion between the clusters is characterized by an inter-particle friction coefficient which was determined using the angle of repose of a pile of powder with a given particle size. Details of this method have been described in [9].

5. Conclusions

Three dimensional imaging was used to capture the shape and size distribution of coke aggregates. Modeled coke aggregates were used to investigate the packing density and electrical resistivity of coke particle mixes by means of discrete element method. Determining the pore size distribution in the sample with only coarse particles was performed through void tracking on the numerical model of S5. An industrial aggregate recipe of coke aggregates for making anode paste was then modified according to the results of void tracking. The modified recipes have higher content of coarse particles and fewer fines but their vibrated bulk density is comparable to standard sample. Electrical resistivities of the samples were also measured. Results showed that modified recipes not only provide a comparable or better bulk density but they have a smaller electrical resistivity as well. DEM investigations on inter-particle contacts show that reducing the amount of fine particles decreases the contact density and increases the average contact radius within the sample. These two effects, if the bulk density is not compromised, result in a lower electrical resistivity.

6. References

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