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# Discrete Element Method Applied to the Vibration Process of Coke Particles

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## Abstract

Physical properties of coke particles including particle shape and size distribution have direct effects on their packing density. In the present work, effects of particle shape and size distribution on vibrated bulk density (VBD) of dry coke samples have been investigated. Discrete Element Method (DEM) has also been used to simulate the vibration process. Results showed that the shape and size distribution of particles influence the bulk density of coke and these parameters can be used to describe the packing density of coke particles. In general, mixed samples provide higher VBD than mono-size samples and as the fraction of coarse particles increases vibrated bulk density increases. However, existence of 10 wt.% of fine particles to fill the pores between coarse particles is essential. Simulation results were also reasonably consistent with experimental data. Finally, it is noteworthy that a well–tailored DEM model is capable of predicting the particle rearrangement and density evolution during the vibration process.

## Introduction

Consumable carbon anodes are used in Hall-Héroult process. Quality and properties of anodes have a considerable effect on the efficiency of electrolysis cells [1]. Carbon anodes are produced by mixing granulated calcined petroleum coke and coal tar pitch, pressing and baking the obtained paste. Physical and chemical properties of raw materials influence the quality of the anodes. Porosity of calcined coke is an important parameter in carbon anode production which is used in determination of pitch demand [2,3,4]. It has been shown that increasing the bulk density of coke enhances the baked apparent density [2,5] and also reduces the air permeability [6] of the anodes. Parameters which affect the bulk density of coke include the shape, size, and size distribution of coke particles. Vibrated Bulk Density (VBD) of calcined cokes is also related to properties of green coke such as Hardgrove Grindability Index (HGI) and volatilies content [7]. Dion et al.[7] showed that as the calcination temperature of coke increases from 1100 to 1300°C the VBD of coke increases. However, exact effects of shape and size distribution of coke particles especially in the range that are widely used in anode plants are not fully understood and need further investigations.

The present work attempts to evaluate the effect of size distribution of coke particles on VBD of calcined cokes. Numerical simulation using the Discrete Element Method (DEM) is applied to modelling the coke particles during the VBD test.

## Discrete Element Method

Discrete Element Method introduced by Cundall and Strack [8] in 1979, has been used in several investigations to simulate the behavior of granular materials in industrial applications, especially where the dynamics and flow of a particulate material is of interest. In DEM simulations, the material is discretized using rigid elements, spheres in 3D and circles in 2D models. Mechanical behaviour of the material is modeled by defining the contact properties between the elements. A classical explicit time integration scheme is used.

At the beginning of each time step, the active contacts are determined according to known positions of all elements and walls. Then, by applying the force-displacement law to each contact, the contact forces are updated. Finally, law of motion is applied to each particle, and position and velocity of all particles are updated. Hence, it could be said that the main part of a DEM model is the definition of contact model and contact properties, which in turn determine the mechanical response of the material. One common contact model which is widely used in DEM simulations is termed linear contact. This model is simply defined by assigning the values of normal and shear stiffnesses to the contacting elements (see Figure 1). Normal and shear stiffness of the contact are expressed as follows in which $K_A^n, K_A^s, K_B^n$ and $K_B^s$ are normal and shear stiffness of particle A and B respectively.

$$K^n = \frac{K_A^n . K_B^n}{K_A^n + K_B^n} \quad (1)$$

$$K^s = \frac{K_A^s . K_B^s}{K_A^s + K_B^s} \quad (2)$$

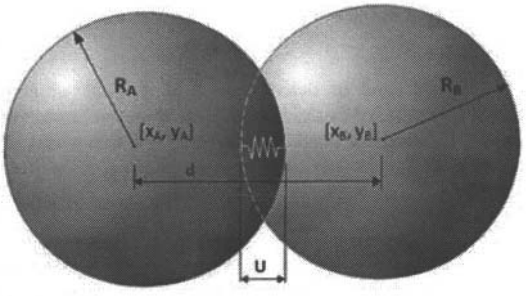


**Figure 1. Contact of two elements**

Having the shear and normal stiffnesses, contact forces can be calculated according to the extent of overlapping, $U^n$,(for normal contact force) and tangent movement, $\delta U^s$(for shear contact force);

$$F^n = K^n . U^n \quad (3)$$

$$F^s = -K^s . \delta U^s \quad (4)$$

**Numerical Model**

The discrete element method in this work is used to model the coke particle assemblies. However, the fundamental elements in two-dimensional DEM model are circles. Thus, real shape coke particles should be modeled using overlapping circles to be used in the DEM model. Coke particles in the size range of -6+14 mesh areshown in Figure 2. The image processing toolbox of Matlab was used to generate models of particles. As can be seen in Figure 3, the real shape of coke particles can be modeled by overlapping circles.

Mass of an irregular shape particle (clump) is defined by the sum of the masses of its constituent balls;

$$m^{Cl} = \sum_{n=1}^{N_b} m^{[n]} \quad (5)$$

in which $m^{Cl}$, $N_b$ and $m^{[n]}$is the mass of the clump, number of the balls of the clump and the mass on the $n$th ball respectively. Volume of the clump is obtained by deducting the overlaps from the sum of the volumes of its constituent balls. Density of individual balls assigned in a way that the total density of the clump matches the original coke particle. The center of mass of a clump is also determined from the mass and position of all balls within that clump.

$$x_i^{Cl} = \frac{1}{m^{Cl}} \sum_{n=1}^{N_b} m^{[n]} x_i^{[n]} \quad (6)$$

Moments and products of inertia, $I_{ii}$ and $I_{ij}$, for a clump can also be calculated as follows;

$$I_{ii} = \sum_{n=1}^{N_b} \{ m^{[n]} \left( x_j^{[n]} - x_j^{Cl} \right) \left( x_j^{[n]} - x_j^{Cl} \right) + \frac{2}{5} m^{[n]} r^{[n]} r^{[n]} \} \quad (7)$$

$$I_{ij} = \sum_{n=1}^{N_b} \left\{ m^{[n]} \left( x_i^{[n]} - x_i^{Cl} \right) \left( x_j^{[n]} - x_j^{Cl} \right) \right\}; \quad i \neq j \quad (8)$$

These data are used in determination of motions of clumps. Clumps are considered as rigid bodies and, therefore, translational motion of the center of mass and the rotational movement of the entire clump define the motion of a clump.

$$F_i = m\left(\frac{\partial^2 x_i}{\partial t^2} - g_i\right) \quad (9)$$

The force in Equation (9) is the sum of externally applied forces on the clump (such as the vibrational force by the container wall), as well as the body force and forces from the contacts. The equation of motion (9) is integrated by a finite difference method, and translational and rotational accelerations can be calculated as follows:

$$\ddot{x}_i^{(t)} = \frac{1}{\Delta t}\left( \dot{x}_i^{\left(t+\frac{\Delta t}{2}\right)} - \dot{x}_i^{\left(t-\frac{\Delta t}{2}\right)} \right) \quad (10)$$

$$\dot{\omega}_i^{(t)} = \frac{1}{\Delta t}\left( \omega_i^{\left(t+\frac{\Delta t}{2}\right)} - \omega_i^{\left(t-\frac{\Delta t}{2}\right)} \right) \quad (11)$$

The stability of finite difference solution depends on the time-step ($\Delta t$) which is in turn a function of the mass and stiffness of the particles. For dynamic problems such as the problem in this work, the time-step becomes very small (around 2e-6 seconds) and it makes the simulation computationally expensive.

Vibrated Bulk Density testing of calcined cokes was conducted according to ASTM D4292. The setup has a cylindrical container which can have a vibration of amplitude of 0.2 mm with frequency of 60 Hz. Duration of the test is 1 minute. Six kinds of coke samples as given in Table 1 were used in this investigation. Coke particle models (obtained by image processing) were used in a two dimensional simulation of the VBD test by Particle Flow Code, PFC2D software (Itasca Consulting Group Inc.). For each size range, three particles were modeled and total mass of particles for each modeled sample was 100 mg.

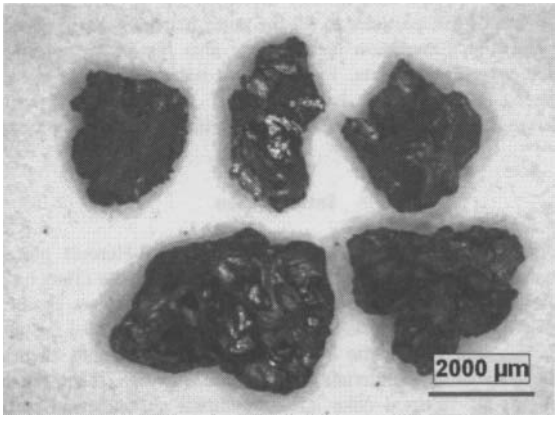


**Figure 2. Micrograph of coke particles in the size range of -6+14 mesh**

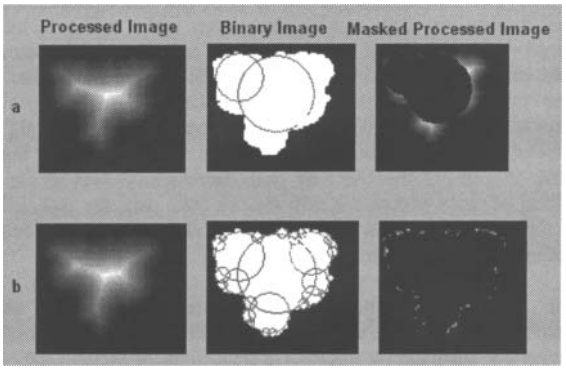


**Figure 3. Image Processing by Matlab and modeling the irregular-shape coke particle by circles. a) covering the area by two circles b) the particle has been modeled using 26 circles**

It is worthy to emphasize that two dimensional modeling in this study has been used due to ease of application. Therefore, it is a qualitative work aimed to understand the mechanisms of irregular-shaped particle packings and effects of shape and size of coke particles on the VBD of coke powders.

## Results and Discussions

Six coke powders with the particle size distributions as given in Table 1 were modeled. Particles were placed at random positions inside the container and then they were settled by applying the force of gravity.. The equilibrium state in this work was defined when the ratio of the maximum unbalanced force to the maximum contact force is less than 1e-5. Then vibrational force was applied to the container for 60 seconds.

Experimental results of the VBD test and also those obtained from DEM simulations have been shown in Figures 4 and 5. Figure 4 shows the VBD values for mono-size range powders (S1, S2 and S3). As it could be seen, changing the particles size from the mesh size range of -30+50 to -14+30 did not have a visible effect on the VBD value (0.910 g/cm$^3$ for both).

**Table 1. Particle size distribution of the coke samples. Weight percentage of each size range has been given.**

| Samples | Mesh Size range | | |
|---|---|---|---|
| | -30+50 | -14+30 | -6+14 |
| S1 | 100% | - | - |
| S2 | - | 100% | - |
| S3 | - | - | 100% |
| M1 | 50% | 40% | 10% |
| M2 | 30% | 40% | 30% |
| M3 | 10% | 40% | 50% |

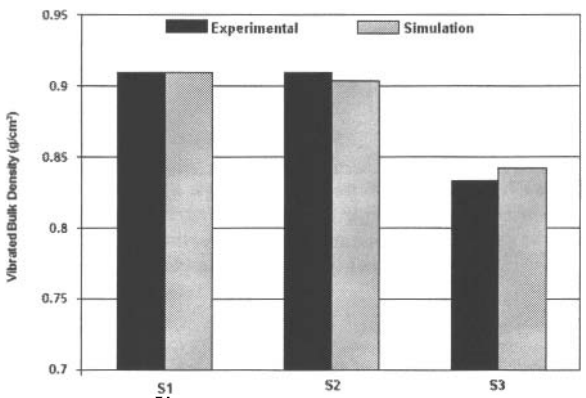


**Figure 4. VBD values for mono-size samples and comparison of experimental data and simulation predictions**

However, increasing the particles size to the range of -6+14 mesh reduces the VBD to 0.834 g/cm$^3$. The container diameter is 30 mm. The diameter of the largest particles is 3.3 mm and the smallest particles which correspond to -30+50 mesh range, have a

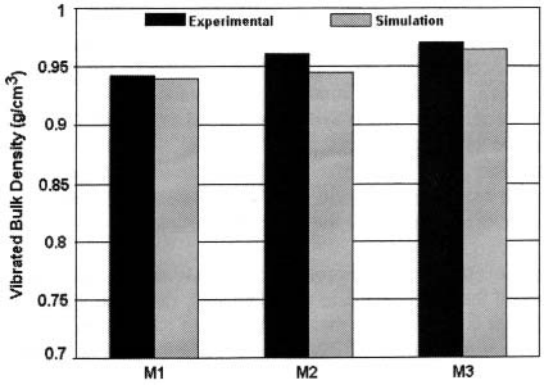


**Figure 5. VBD values for mixed samples and comparison of experimental data and simulation predictions**

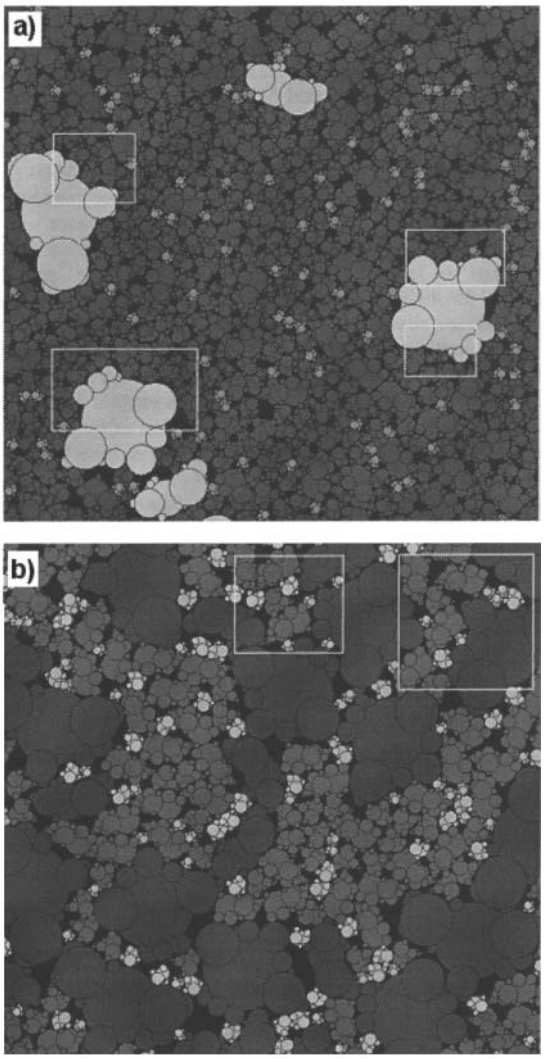


**Figure 6. Simulation of particle packings; a) sample M1, filling the surface roughness of coarse particles by fines are shown by rectangles b) sample M3, the indicated areas show the filling of the space between large particles by fines**

diameter of 0.3 mm. The exact reason of the difference in the obtained values of the VBD is not clear. However, there are some parameters that can affect the packing density of the particles. It has been shown that container wall induces a region of low density and this effect is more pronounced for the larger particles and the low density region size is equal to around 10 particle diameters [9]. The simulations of VBD tests for samples S1, S2 and S3 as shown in Figure 4 follow the same trend and give the minimum value of VBD for the coarse particles.

On the other hand, microscopic studies of the coke particles showed that as the particle size increases, the mean sphericity of particles decreases. The mean sphericity of particles in S1, S2 and S3 samples was 0.804, 0.794 and 0.4. Therefore, lower VBD of S3 compared to S1 and S2 could be also due to particles shape (lower sphericity) within the size range of -6+14 mesh.

Results of simulation predictions and also experimental data for the mixed samples (M1, M2 and M3) have been plotted in Figure 5. It can be seen that as the content of coarse particles increases the VBD increases. The sample M3 has more coarse particles and less fines compared to M1 and M3 and it holds the maximum VBD in this investigation. Figure 4 shows that coarse particles have lower packing density whereas Figure 5 suggests that increasing the content of coarse particles leads to higher VBD. It should be noted that the results in Figure 4 are for mono-size particles while Figure 5 presents the data for mixed samples.
Images from the simulations may be helpful to understand the mechanisms of particle packing. Images of coke particle assemblies for the mixed samples of M1 and M3, obtained from simulations, are shown in Figure 6. For the sample M1 ( Figure 6.a) coarse particles of -6+14 mesh range make up only 10 wt.% of the sample. However, for the sample M3, 50 wt.% are coarse particles. Comparing figures 6.a and 6.b can explain the higher bulk density of M3 compared to M1. Formation of inter-particle porosity between fines (as indicated by rectangular areas in figure 6.a) seems to be the reason for lower VBD of sample with higher percentage of fine particles. As can be seen in figure 6.b, increasing the content of coarse particles leads to formation of less inter-particle spaces.

However, it should be noted that the size of fine particles here is small enough to fill the surface roughness of coarse particles and also the voids between large particles.
Porosity measurements in different regions of the particle assemblies showed that the mean porosity value in areas with fine particles is around 15.4% while it is 10.8% for the same area around a large particle.

Although coarse particles have positive effect on the bulk density, it should be noted that existence of fines to fill the gaps between large particles (as shown in Figure 6.b) is necessary. Comparing the graphs in Figures 4 and 5 shows that the maximum value of VBD is not for S3 sample (having 100% of large particles) or sample S2 (with 100% of medium size particles).

Another parameter which affects the particle packing densities is the container wall effect. It is believed that the ratio of container size to the particle size is also an important parameter in packing density of granular materials [9]. The container wall induces a local low density region nearby which reduces the total packing density of the material. This effect is more pronounced when the particle size increases (in the same container). As can be seen in Figure 7.a, there are large voids between the particles close to the container wall which can explain the lower density of S3 compared to S2 and S1. However, these voids have been filled by fine particles in sample M3 (Figure 7.b).Therefore, it can be said that coarse particles have a positive effect on the vibrated bulk density and increasing the coarse particle fraction increases the VBD, if there are enough fines to fill the gaps between large particles.

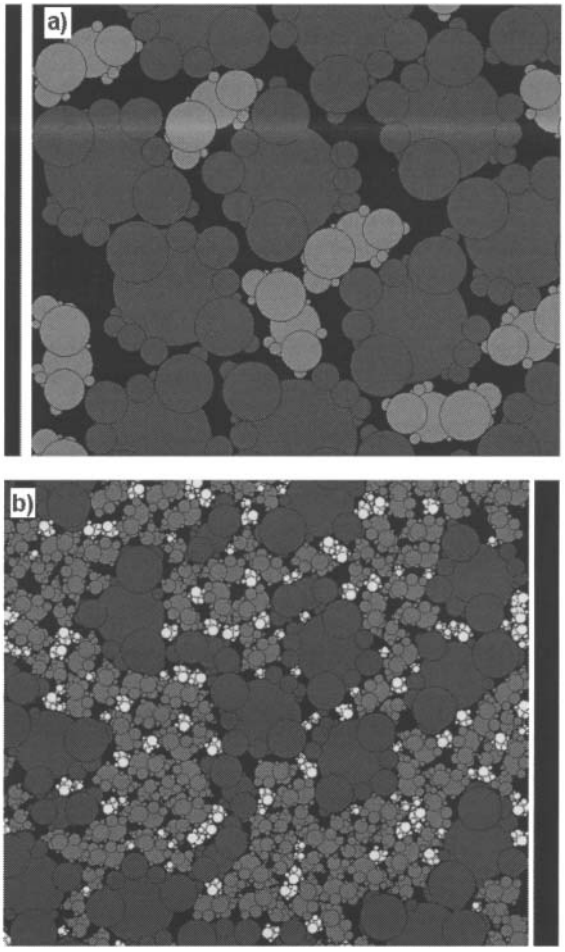


**Figure 7. Simulation of particle packings; a) Regions near the container wall in sample S3, filling the surface roughness of coarse particles by fines are shown by rectangles; b) Regions near the container all in sample M3**

## Conclusions

Vibrated Bulk Density of calcined cokes has been investigated. The Discrete Element Method using PFC2D has also been applied to simulate the VBD test. Results confirmed that VBD of cokes is affected by the size and shape of particles. For mono-size samples within the investigated size range, the maximum and the minimum VBD values correspond to the samples in the range of -30+50 and -6+14 mesh respectively. It is believed that the wall effect and lower sphericity (0.4) of S3 particles compared to S2 and S1 (0.794 and 0.804 respectively) are the main reasons for the

lower VBD value of S3. In general the mixed samples have more bulk density than mono-size ones. It could be concluded that in the investigated size range, as the fraction of coarse particles increases, VBD increases only if there are fines to fill the pores between large particles. Finally it should be emphasized that the present work is a two-dimensional simulation of VBD test of coke samples and helps to understand the effects of parameters such as size, size distribution, and shape of particles on the VBD value. To obtain precise quantitative data, three-dimensional simulations are recommended.

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