

A Numerical Analysis of the Mechanical Behavior of Coke Aggregates under Monotonic and Cyclic Loadings

Alireza Sadeghi Chahardeh¹, Roozbeh Mollaabbasi², Donald Picard³, Seyed Mohammad Taghavi⁴ and Houshang Alamdari⁵

1. Ph.D. candidate of Aluminum Research Centre–REGAL
2. Postdoctoral researcher
5. Professor

Aluminum Research Centre–REGAL, Mining, Material, and Metallurgy Engineering Department, Université Laval, Québec, Canada.

3. Application specialist of Eddyfi Technologies Company, Québec, Canada.
 4. Professor of Chemical Engineering Department, Université Laval, Québec, Canada.
- Corresponding author: houshang.alamdari@gmn.ulaval.ca

Abstract

Carbon anodes are part of the chemical reaction to reduce alumina in the Hall-Héroult process, of which coke aggregates make up a major part (about 85%). The study of the mechanical behavior of coke aggregates not only leads to a better understanding of the deformation mechanisms of granular materials under a compressive loading, but also can identify potential causes of structural defects in carbon anodes, such as horizontal cracks. On the other hand, thanks to recent advances in high performance computing, it is possible to simulate the behavior of granular materials such as coke aggregates with respect to the interactions between particles. Therefore, in this work, we investigate the most important factors affecting the mechanical behavior of granular materials, such as the particle size distribution as well as the rolling resistance between the particles, a parameter considering the particle shape through the discrete element method (DEM) modeling. Considering carbon anodes produced by the vibrocompaction process, the effects of frequency and number of cycles of this process on the final density of the coke mixture are investigated. The results reveal that by adding the small particles to the mixtures, the reversible deformation decreases through the monotonic loading condition. In addition, increasing the rolling resistance decreases the amount of permanent deformation in the monotonic loading condition. On the other hand, by increasing the frequency of vibrocompactor, the permanent deformation is enhanced. Moreover, a comparison between monotonic and cyclic loading conditions states that, although increasing the strain rate reduces the permanent deformation in the monotonic loading, in the cyclic loading, increasing the strain rate increases the permanent deformation.

Keywords: Carbon anode, Discrete element method simulation, Monotonic loading, Cyclic loading.

1. Introduction

Carbon-like materials such as the anode and the ramming paste are crucial parts of electrolysis cells in the Hall-Héroult process. It is shown that 6.5% of the voltage drop across the cell is due to the voltage drop associated with the anode assembly [1]. Anode quality characteristics, such as density, electrical resistance and reactivity affect not only the energy efficiency of aluminum production but also the amount of carbon consumed and the resulting environmental concerns [2]. The carbon anodes are composed of two major parts, i.e., the dry coke aggregates (85 wt.%) and the coal tar pitch (15 wt.%). Due to the limited resources for anode fabrication, changes in the properties of raw materials, and consequently the parameters of the anode production process, consistent, homogeneous, and high-quality anode production are a major challenge for the anode fabrication. It should be noted that the main parameters of the anode vibrocompaction process are the amount of pressure, speed, duration of formation, and the temperature of the process.

Coordination of the anode production parameters with new raw materials is another problem of carbon anode production.

The carbon anodes in most aluminum smelters are produced by the vibration compression process. It has been shown that the anodes produced in this process have a higher quality compared to the monotonic compaction process [3]. Azari et al. investigated the effects of raw materials, such as particle shape and coke/pitch ratio, on the mechanical behavior of green anodes during the monotonic compaction [2, 4]. Thibodeau et al. determined the mechanical behavior of anode paste during the compaction process at 150 °C using the monotonic and cyclic compaction tests [5]. Based on the experimental results, they showed that a small axial stress level in the quasi-static regime leads to a significant compression of the green anode before skeletal formation. After that, the stress required for additional compaction increases. In addition, by performing cyclic compaction experiments with a linear loading/unloading rate (0.2 MPa/s) on the dry coke aggregates, Thibodeau et al. emphasized that a combination of hardening-softening behavior during each loading cycle [6]. Based on the results of experiments on the anode paste, Kansoun et al. investigated the mechanical behavior of a commercial-grade carbon paste used in the aluminum industry during the monotonic and cyclic compaction tests [3]. They showed that the stress required for the anode compaction at the cyclic loading is less than the monotonic one. On the one hand, they claimed that the strain rate does not affect the anode paste behavior in the quasi-static regime. On the other hand, they declared that the strain rate plays a negative role in the dynamic regime compression of anode paste. It means that for reaching the target density, more pressure is needed. Extensive research has also been done on the mechanical behavior of hot asphalt mixtures, which have a similar composition to anode paste mixtures [7]. Accordingly, the mechanical behavior of asphalt mixtures under cyclic loads includes important phenomena such as (1) hardening-relaxation behavior, (2) particle rearrangement, and (3) the permanent deformation due to cyclic loads is significantly greater than the permanent deformation due to monotonic loads [8]. However, investigation of production parameters affecting the anode quality through laboratory tests has problems such as opacity of the anode paste and high temperature of the production process [9, 10]. Hence, the numerical modeling of carbon anode paste can be considered as a practical solution.

Many attempts have been made to model the mechanical behavior of the anode. Chaouki et al. have proposed a constitutive law to simulate the anode paste during the compaction process [11]. Although this model can reveal the density gradient due to the stub-hole, it is not capable of demonstrating the formation of localized bands [12]. It should be noted that localized bands refer to an area of the material that has undergone non-uniform deformation, in that the deformation is mainly concentrated in it [12]. This limitation stems from the fact that the granularity nature of the anode paste cannot be considered by phenomenological models such as finite element methods [13]. Moreover, many research works have been done to investigate the behavior of anode paste using the discrete element method (DEM), which considers grains as the basic element from which the mechanical behavior of granular materials originates [14]. DEM has shown the ability to successfully simulate some properties of the anode coke aggregates, such as the bulk density [15] and the electrical resistivity [16].

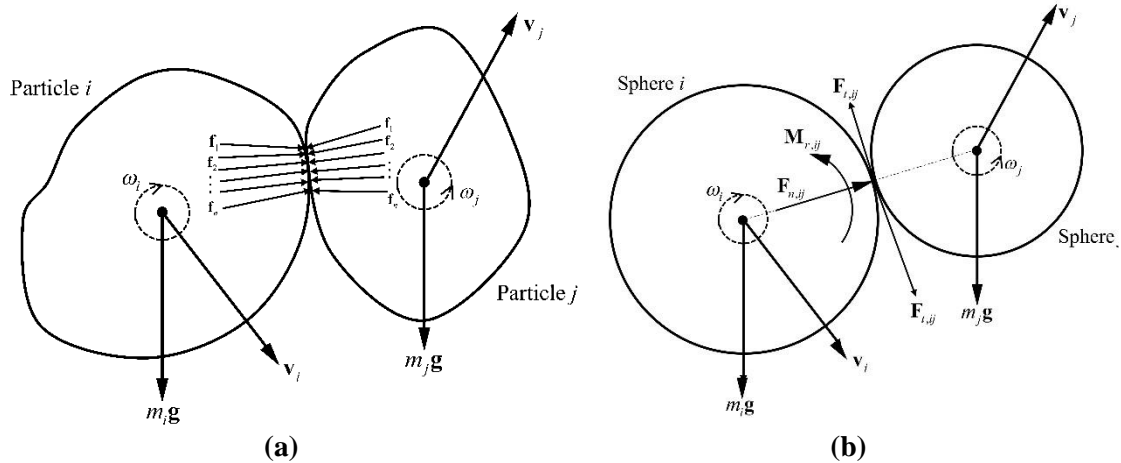


Figure 1. The interaction between (a) two real particles and (b) two spheres in DEM (m_i is the mass of particle i , g is the gravitational acceleration, $F_{(t,ij)}$ is the tangential contact force between the particles, $F_{(n,ij)}$ is the normal contact force between the particles, $M_{(r,ij)}$ is the rolling moment between the particles, f_n is the force interaction between the particles, v_i is the linear velocity, and ω_i is the angular velocity).

In this paper, the mechanical behavior of coke aggregates under the cyclic and monotonic loadings are investigated through a DEM modeling approach. Since coarse coke particles have been shown to form a skeleton that controls the main mechanical behavior of coke aggregates [6], in this paper only coarse coke aggregates are considered. In Section 2, the concept of the DEM with rolling resistant effect is reviewed. In Section 3, the mechanical behavior of the coke aggregates, both in the monotonic and cyclic loading conditions will be investigated. Section 4 will summarize and discuss the most salient results of this work.

2. Material and Methods

2.1 Discrete Element Method

DEM was introduced by [17] to simulate the mechanical behavior of granular materials in which the particles are considered essential components. Many attempts have been made to model the behavior of anode paste using DEM. Although the modeling of the coke aggregate compaction involves complexities such as different size distributions, particle shapes, and solid-fluid interactions, it has been shown that DEM can successfully simulate some properties of granular materials, such as the mechanical and failure behaviors [13, 14]. Therefore, DEM has shown that it has many capabilities in providing a realistic model of coke aggregate samples.

Let us consider two particles i and j with arbitrary shapes (see Figure 1 (a)) that are in contact with each other on a surface, and force interactions between them (f_1, f_2, \dots, f_n). Now, assume these two particles are replacing by two spheres with radii R_i and R_j ; to be able to consider the effects of these force interactions, we can apply a rolling moment ($M_{r,ij}$) at the point of contact of the two spheres in addition to the normal ($F_{n,ij}$) and tangential ($F_{t,ij}$) contact forces. This rolling moment, in addition to replacing the role of force interactions between the particles, can also be a parameter of the shape of the particles that prevents their free rotation. Therefore, the motion of particle i is governed by the Newton-Euler equations as follows:

$$\begin{aligned}
 m_i \mathbf{g} + \sum_{j=1}^{N_i} \mathbf{F}_{n,ij} + \sum_{j=1}^{N_i} \mathbf{F}_{t,ij} &= m_i \frac{d\mathbf{v}_i}{dt}, \\
 \sum_{j=1}^{N_i} \mathbf{M}_{r,ij} &= I_i \frac{d\omega_i}{dt},
 \end{aligned} \tag{1}$$

where N_i is the number of contacts, m_i is the particle mass, and I_i is the principle moment of inertia. In addition, the normal ($\mathbf{F}_{n,ij}$) and tangential ($\mathbf{F}_{t,ij}$) contact forces as well as the rolling resistance moment ($\mathbf{M}_{r,ij}$) are characterized by

$$\begin{aligned}
 \mathbf{F}_n &= K_n \delta_n, \\
 \Delta \mathbf{F}_t &= -K_t \Delta U_t \quad \text{with} \quad \|\mathbf{F}_t\| \leq \|\mathbf{F}_n\| \tan \phi_c, \\
 \Delta \mathbf{M}_r &= -K_r \Delta \theta_r \quad \text{with} \quad \|\mathbf{M}_r\| \leq \|\mathbf{F}_n\| \eta_r \min(R_i, R_j),
 \end{aligned} \tag{2}$$

where K_n , K_t , and K_r represent the constant normal stiffness, the constant tangential stiffness, and the constant of rolling stiffness, respectively; ϕ_c is the contact friction angle; η_r is the coefficient of rolling friction; δ_n is the overlapping distance between spheres; U_t is the relative tangential displacement at the contact point; and θ_r is the relative rolling rotation of particles. The constants of stiffness are defined from an elastic modulus, E , and dimensionless tangential and rolling coefficients, α_t and α_r , respectively:

$$K_n = 2E \frac{R_i R_j}{R_i + R_j}; \quad K_t = \alpha_t K_n; \quad K_r = \alpha_r R_i R_j K_t. \tag{3}$$

The rolling resistance model is phenomenologically developed to produce a larger simulated shear strength [18]. In other words, by considering this model, it is possible to simulate a phenomenon in which the particles have less rotation due to the effect of their shape. Hosn et al. [19] numerically showed that the plastic macroscopic behavior of the granular material is a function of the plastic parameters at the microscopic scale (ϕ_c and η_r) and mainly corresponds to the plastic rolling moment ($\|\mathbf{F}_n\| \eta_r \min(R_i, R_j)$), reflecting the particle's shape. Therefore, the main parameter for considering the particle shape effect is η_r , and the dimensionless rolling coefficient α_r does not affect the plastic macroscopic behavior of the granular materials [19]. By comparing the overlapped sphere model and the rolling resistance model, Sadeghi-Chahardeh et al. [13] demonstrated that the rolling resistance can be used as a parameter representing the shape of the particles in DEM modeling.

2.2 Simulation Setup

In this paper, the DEM computations are realized using the open-source software YADE [20]. The interactions between the particles are simulated in the normal direction to the contact by a linear elastic spring with a stiffness, K_n , and in the tangential direction by a linear elastic spring with a stiffness, K_t , and the tangential perfect plasticity with a friction angle of $\phi = 18^\circ$. The properties of the materials for the DEM simulations are also given in Table 1. At the beginning of a computational time step, the position of all the elements and the boundaries are known. The contacts are detected by the algorithm according to the known position of the elements, and the magnitude of the possible overlaps between the elements calculated by the interaction law (Equation 1). After that, the forces are measured according to the law of motion for each particle, and the velocity and acceleration of the particles are calculated. Then, the new sphere positions are calculated by applying Newton's second law of motion. The integration time in Newton's second law and the interaction contact law are both carried out by way of an explicit scheme. The

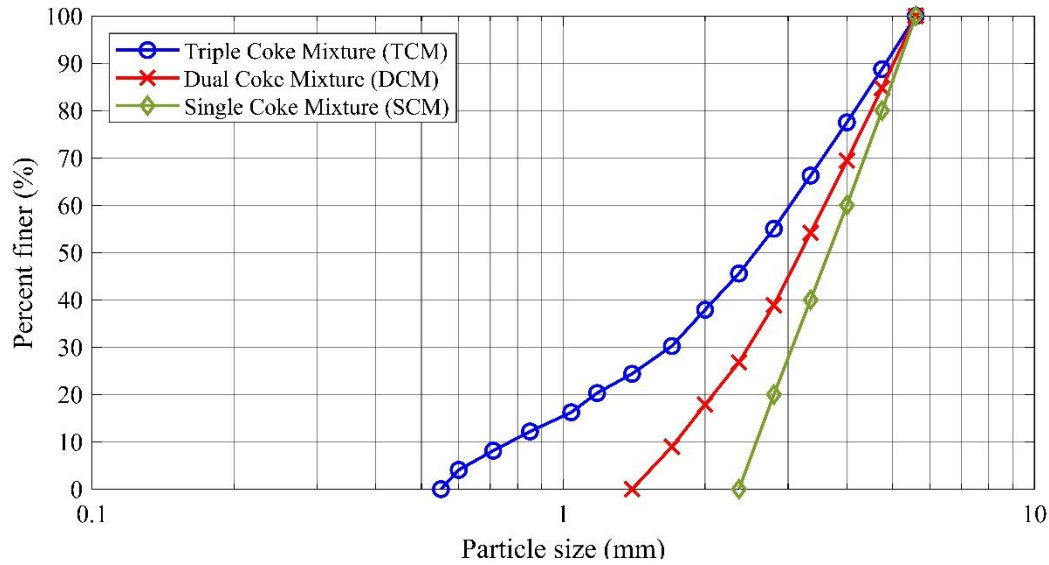


Figure 2. The particle size distribution of the samples.

Table 1. The characteristics of the coke particles used in the DEM model [13].

Property	4-8 US Mesh	8-14 US Mesh	14-30 US Mesh
Density (kg/m ³)	1377	1523	1523
Elastic modulus (MPa)	681	681	681
Poisson ratio	0.3	0.3	0.3
Friction angle (rad)	0.31	0.31	0.31
Damping ratio	0.4	0.4	0.4
Dimensionless of tangential coefficient	0.385	0.385	0.385
Dimensionless of rolling coefficient	2	2	2
Coefficient of rolling friction (η_r)	0.1	0.1	0.1

positions of all particles and the boundaries in the current time step are determined by the obtained values. This cycle of the calculations is repeated and solved at each time step, and thus the flow or the deformation of the material is simulated.

2.3 Sample Creation

The coke aggregate sample in this paper is generated by randomly inserting the particles within a cylindrical domain ($D = 49.8$ mm) and applying gravity to the particles to naturally compact them. The boundaries of the cube are assumed to be displacement-controlled and frictionless. Therefore, the interaction of the particles and the boundaries of the cube will be in the normal direction of their contacts. The boundaries of the cube in the lateral directions (X and Y axes) and its bottom are fixed. The number of particles in the samples are shown in Table 2 and the particle size distributions are depicted in Figure 2. The samples are then compacted by a frictionless movable wall in the axial direction until the samples reach the desired porosity.

It should be noted that the weight of the samples are the same and equal to 250 g. The pre-compression response of the sample is depicted in Figure 3. The velocity of the wall in the pre-compression process, both in the loading and the unloading, is equal to 10 mm/s. This figure shows how to reduce the sample height (increase the sample density) at the end of the pre-compa-

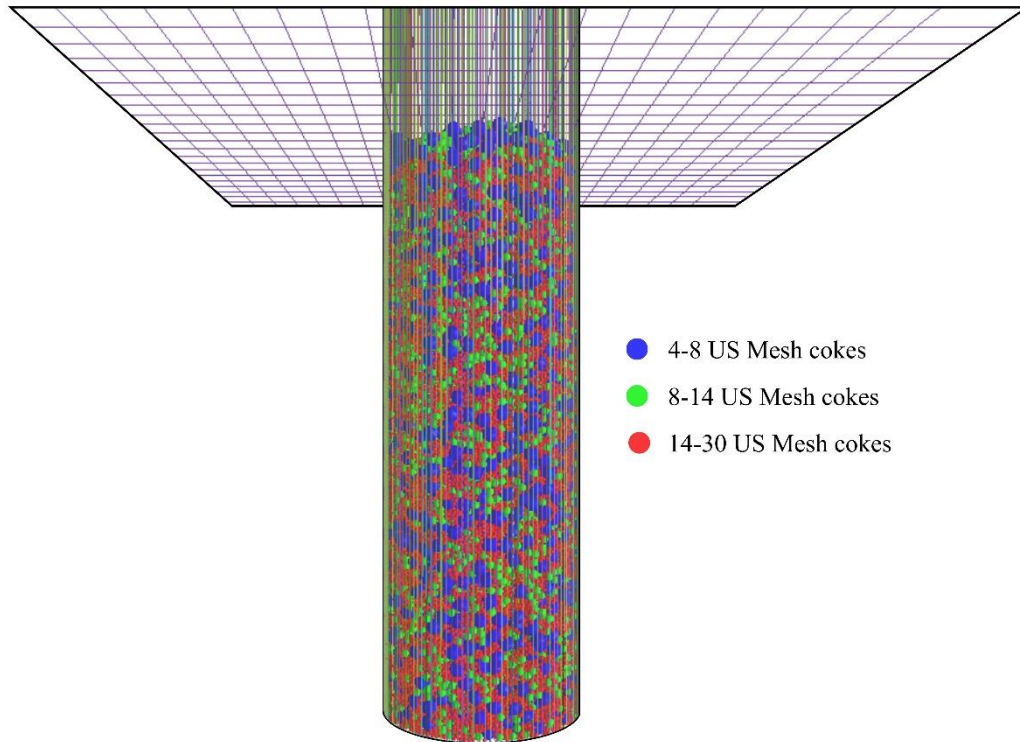


Figure 3. The sample in the DEM simulation of coke aggregates (TCM sample).

Table 2. The number and distribution of coke particles in the samples.

Name of mixture	4-8 US Mesh ($d_{ave} = 3.7$ mm)	8-14 US Mesh ($d_{ave} = 1.7$ mm)	14-30 US Mesh ($d_{ave} = 0.8$ mm)	Total number of particles
Single coke mixture (SCM)	6573 (250 g)			6573 (250 g)
Double cokes mixture (DCM)	4520 (171.9 g)	14306 (78.1 g)		18826 (250 g)
Triple cokes mixture (TCM)	3323 (126.4 g)	10532 (57.5 g)	81778 (66.1 g)	95633 (250 g)

tion process when the external load is removed. It worth to notice that the increase in coke aggregate sample density is due to the rearrangement of the coke particles.

2.4 Monotonic Loading

The purpose of monotonic loading simulations is to investigate factors such as particle size distributions, particle shape and loading speed on the mechanical behavior of coke aggregates during the compaction process. Figure 4 shows the axial loading and unloading of dry coke samples. Both the loading and unloading are linear, and the maximum of the axial stress reaches to 2 MPa. The axial velocity of loading and unloading for investigation of the effect of size distributions and the coefficient of rolling friction, η_r , on the density of coke aggregates is 1 mm/s.

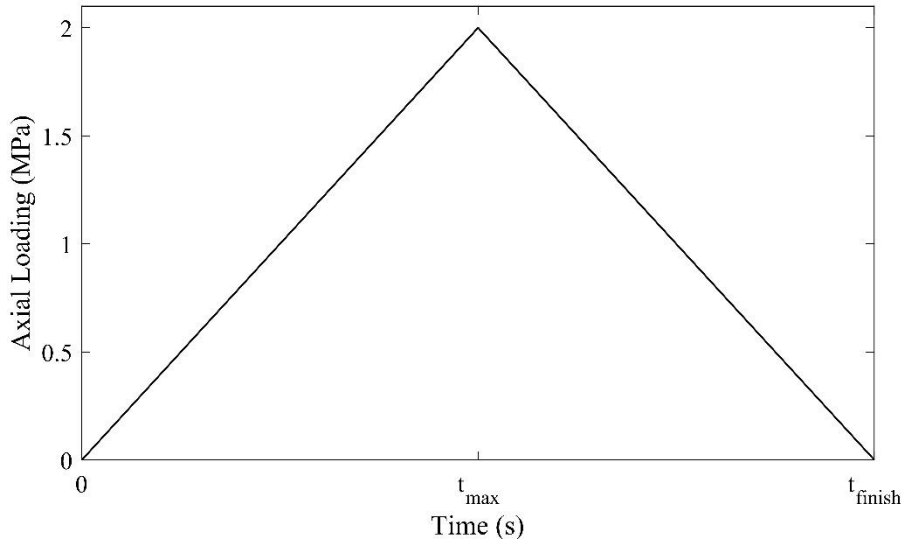


Figure 4. Axial loading during the monotonic loading test.

While, for studying of the strain rate effects, there are three different velocities of 1 mm/s, 10 mm/s, and 50 mm/s. Three different samples for the effect of size distribution on the sample's density are considered (see Table 2). The investigation of the rolling resistance and axial strain rate effects on the density of coke samples are carried out on the triple cokes mixture (TCM).

2.5 Cyclic Loading

These tests aim at investigating the effect of the vibrocompaction frequency and number of cycles on densification and the rigidity of the dry coke aggregates samples. The cyclic loading investigations are performed on the triple cokes mixture (TCM) sample. To this end, vibrocompaction tests were carried out at the following frequencies: 2.96 Hz, 14.79 Hz, and 29.58 Hz. It should be noticed that the frequency of industrial vibrocompactor in the process is about 25 Hz. The samples were subjected to linear loading and unloading that had a maximal amplitude of 2 MPa (see Figure 5).

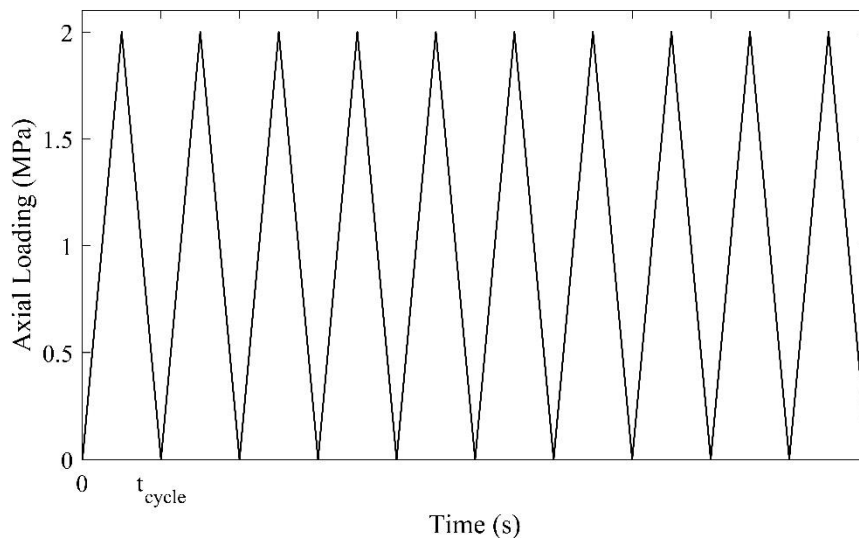


Figure 5. Axial loading during the cyclic loading test.

For the effect of the vibrocompactor frequency, the samples are subjected to 50 cycles of loading and unloading. When the vibrator is stopped, the final height of specimens is calculated, and based

on that, the permanent density of the specimen is calculated. These tests involve linear loading of dry coke aggregates samples, which continue at a constant deformation rate until an axial stress of 2 MPa is reached. An unloading follows and the recoverable deformation is recorded at the end of the unloading. The rigidity modulus is then calculated by dividing the maximum stress of loading by the corresponding recoverable deformation.

3. Results

3.1. Coke Aggregate Response under Monotonic Loading

3.1.1. Effect of Particle Size Distribution

Coke particles of different sizes are used to achieve the required density in the anode paste, so that the smaller particles fill the empty space between the larger particles and increase the contact surface between them. By employing DEM modeling of coke aggregates with different size distributions, Sadeghi-Chahardeh et al. showed that the mechanical behavior of the coke aggregates is strongly influenced by the behavior of larger particles [13]. They found that the smaller particles in the coke mixture are involved in reducing the fluctuations in stress-strain diagram [13].

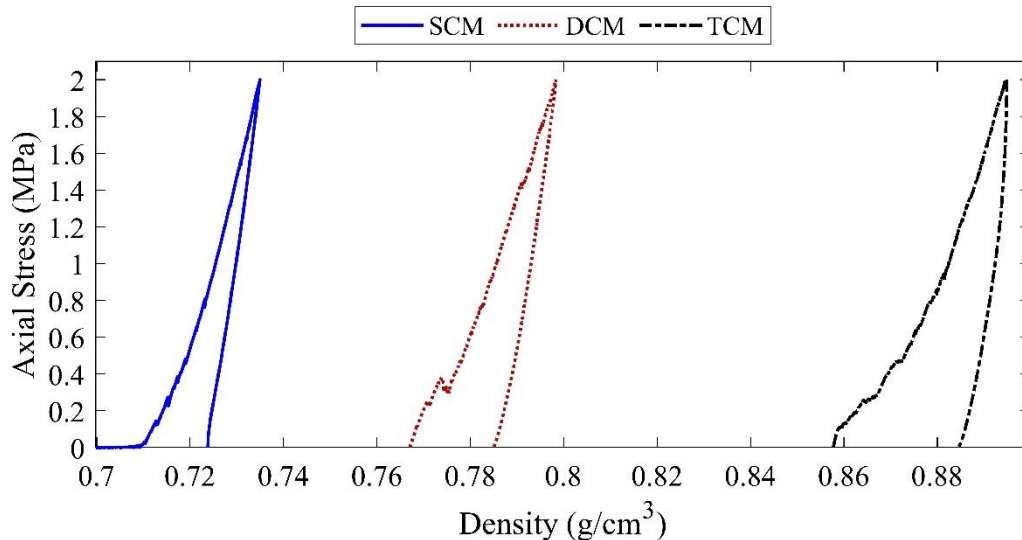


Figure 6. Effect of the particle size distribution on the density of coke aggregates in the monotonic loading (SCM is composed of 4-8 US Mesh coke particles, DCM is composed of 4-8 US Mesh and 8-14 US Mesh coke particles, and TCM is composed of 4-8 US Mesh, 8-14 US Mesh, and 14-30 US Mesh coke particles).

Figure 6 shows the density changes of coke mixture samples with different particle size distributions. As is shown in Figure 6, the smaller particles cause the coke mixture to be denser. Also, with the addition of smaller particles to the coke mixture, the slope of increasing the axial stress is reduced, so that to achieve axial stress of 2 MPa, the sample of TCM, which has 14-30 US Mesh coke particles, undergoes more deformation. The maximum density at the 2 MPa axial pressure for the SCM mixture is 0.737 g/cm³, where the maximum density at the 2 MPa axial pressure for DCM and TCM mixtures is 0.798 g/cm³ and 0.894 g/cm³, respectively. However, when the axial pressure on the top of the samples is removed, the permanent density of samples is calculated. According to Figure 6, the permanent density of the SCM mixture is equal to 0.723 g/cm³. For DCM and TCM mixtures, the permanent density is equal to 0.786 g/cm³ and 0.885 g/cm³, respectively. If the difference between the maximum density and the permanent density is called the reversible density, as shown in Figure 6, the reversible density with adding

the small particles to the mixtures will be decreased. For SCM, DCM, and TCM mixtures, the reversible density is equal to 0.014 g/cm³, 0.012 g/cm³, and 0.009 g/cm³, respectively. In summary, by adding the small coke particles to the coke mixture, the axial pressure required for compression is reduced, the final density is increased and the reversible density of the mixture is reduced.

3.1.2. Effect of Rolling Resistance

The mechanical behavior of the coke aggregates is strongly dependent on the coke particle shapes [13, 21]. By DEM modeling of coke aggregates, Sadeghi-Chahardeh et al. demonstrated that the rolling resistance is a parameter for considering the shape of particles in DEM modeling [13]. Hence, in this section, the effects of the rolling resistance coefficient, η_r , as a parameter of particle shape on the axial stress-density diagram of the TCM mixture are investigated. To achieve this goal, three samples, which are made of a triple coke mixtures (TCM), are taken into account.

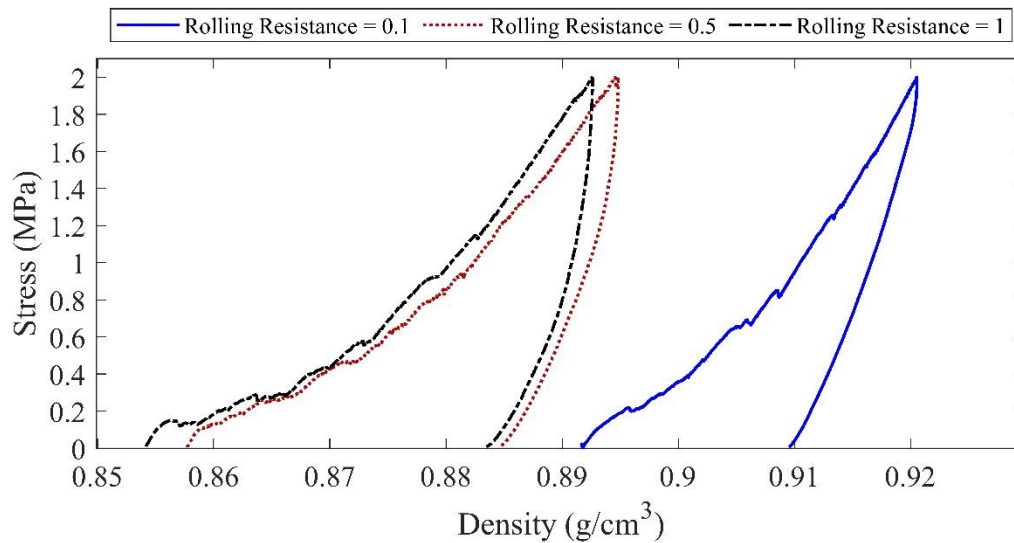


Figure 7. Effect of the rolling resistant coefficient, η_r , on the density of the triple coke mixture (TCM) in the monotonic loading.

Figure 7 presents the axial stress-density diagram of the samples. The higher rolling resistance coefficient and consequently higher amount of rolling moment can be considered as an indication that the particles have a more complex geometry and move away from the spherical state. According to Figure 7, by increasing the coefficient of rolling friction, the densification ability of samples decreases. As a result, both the maximum density at the axial pressure of 2 MPa and the permanent density decrease. The maximum density of the samples with the rolling resistance coefficient of 0.1, 0.5, and 1 are equal to 0.921 g/cm³, 0.894 g/cm³, and 0.892 g/cm³, respectively. Moreover, the permanent density of the samples with the rolling resistance coefficient of 0.1, 0.5, and 1 are equal to 0.91 g/cm³, 0.884 g/cm³, and 0.883 g/cm³, respectively. Therefore, the reversible density for those samples can be calculated. The reversible density for the samples with the rolling resistance coefficient of 0.1, 0.5, and 1 are equal to 0.011 g/cm³, 0.010 g/cm³, and 0.009 g/cm³, respectively. Therefore, by increasing the rolling resistance coefficient, which means that the particles have a more asymmetric geometry, the reversible density will decrease. The reversible density can be used as a parameter for the spring back of materials. Hence, it can be concluded that when the coke particles have a more complex geometry (or they apply higher rolling moments to the neighboring particles), the spring back of the coke mixture reduces. This may be due to the fact that particles with more complex geometry are better and more locked together, thus reducing the spring back of the coke mixture.

3.1.3. Effect of Strain Rate

Loading speed is always one of the effective parameters in the mechanical behavior of materials with associated flow rules, such as metals [22]. However, the effect of loading rate on the mechanical behavior of materials with non-associated flow rules such as granular materials is not clearly defined. By performing the monotonic compression tests on the anode paste at different speeds (a strain rate range between 0.0074 - 0.74 s^{-1}), Kansoun et al. [3] showed that the anode paste behavior was not strongly dependent on the loading speed in the quasi-static regimes. Contrary, in the dynamic regimes, the density of anode paste is affected by the loading rate, and by increasing the loading speed from 0.37 s^{-1} to 0.74 s^{-1} , the final density of the anode paste reaches from 1.52 g/cm^3 to 1.5 g/cm^3 [3]. In this work, the contribution of coke particles in the effect of loading speed is discussed.

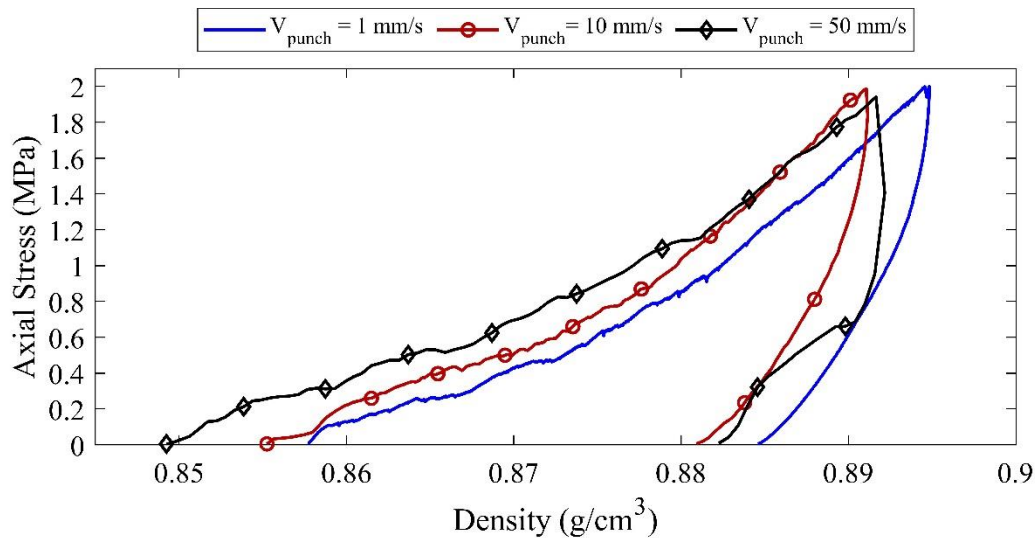


Figure 8. Effect of the strain rate on the density of the triple coke mixture (TCM) in the monotonic loading.

Figure 8 shows the axial stress evolution as a function of the density for loading speed of 1 mm/s , 10 mm/s , and 50 mm/s . The samples are created by the triple coke mixtures (TCM). By increasing the velocity of the loading, the maximum density of the samples decreases. The maximum density for the loading speed of 1 mm/s , 10 mm/s , and 50 mm/s are 0.895 g/cm^3 , 0.8915 g/cm^3 , and 0.892 g/cm^3 , respectively. In addition, the permanent density of the samples for the loading speed of 1 mm/s , 10 mm/s , and 50 mm/s are 0.885 g/cm^3 , 0.881 g/cm^3 , and 0.882 g/cm^3 , respectively. Accordingly, the reversible density for all three loading speeds is almost the same. Therefore, it can be concluded that although velocity has a very small effect on the permanent density of the coke mixture and decreases with increasing velocity, its effect on the amount of reversible density and consequent spring back of the coke mixture sample can be negligible.

Therefore, the results of DEM simulation make it clear that in the compaction process of a granular material, the process speed does not have much effect on the permanent density of the sample. These results are consistent with [3] laboratory results performed on the anode paste.

3.2. Coke Aggregate Response under Cyclic Loading

3.2.1. Effect of Frequency

A series of simulations of vibrocompaction tests were carried out to investigate the effect of the frequency and the number of cycles on the permanent density of the coke aggregates samples.

Recall that the applied load consists of linear stress ranging between 0 and 2 MPa (Figure 5). Figure 9 shows the evolution of the permanent density of the triple coke aggregates sample as a function of the number of the density. The number of cycles for all three frequencies of 2.958 Hz, 14.79 Hz, and 29.58 Hz is 50 cycles. On the one hand, increasing the frequency of the vibrocompactor leads to decreasing the vibrocompaction process time. On the other hand, increasing the frequency means increasing the strain rate during the loadings. It has been shown that increasing the velocity of loading in the monotonic loading condition will decrease the capacity of the material to be compacted. However, increasing the frequency in the cyclic loading conditions has an opposite effect.

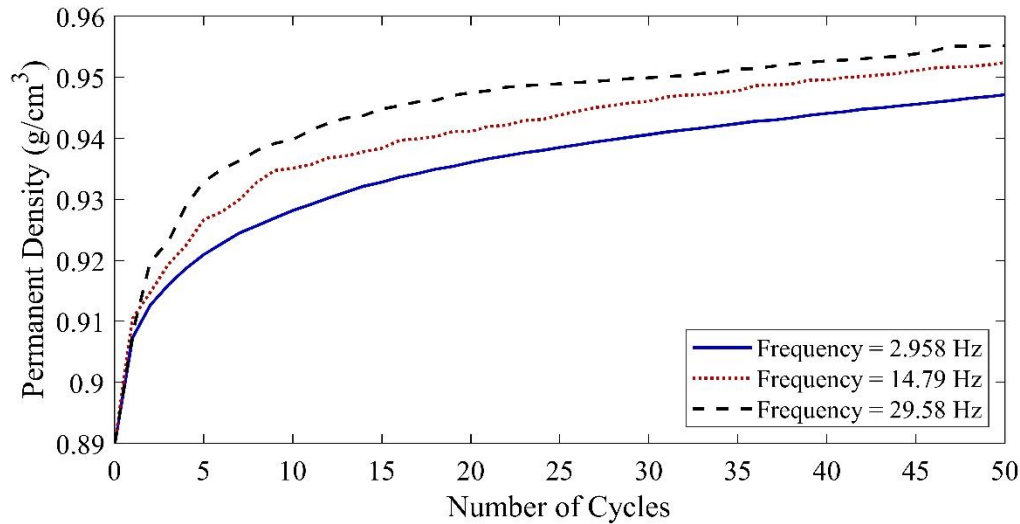


Figure 9. Effect of the loading frequency on the permanent density of the triple coke mixture (TCM) in the cyclic loading.

As is shown in Figure 9, by increasing the frequency the amounts of permanent density increase. The amount of density for the sample with vibrocompaction frequency of 2.958 Hz, 14.79 Hz, and 29.58 Hz is equal to 0.947 g/cm³, 0.952 g/cm³, and 0.956 g/cm³, respectively. Moreover, Figure 9 shows that the slope of the permanent density diagram decreases when the frequency increases. Therefore, it can be deduced that although the permanent density increases with the increasing of the loading frequency, increasing the frequency causes the slope of the permanent density graph to decrease. Thus, after the twentieth cycle, the amount of permanent deformation during each cycle decreases with increasing frequency.

3.2.2. Effect of Number of Cycles

Cyclic loading causes much less force than monotonic loading to achieve the desired density. In the previous section, it has been shown that increasing the frequency increases the permanent density. To investigate the effect of number of cycles on the permanent density, a triple coke mixture that is periodically loaded with a frequency of 14.79 Hz is used. The results are depicted in Figure 10. The permanent density of triple coke mixture increases with increasing of the number of cycles.

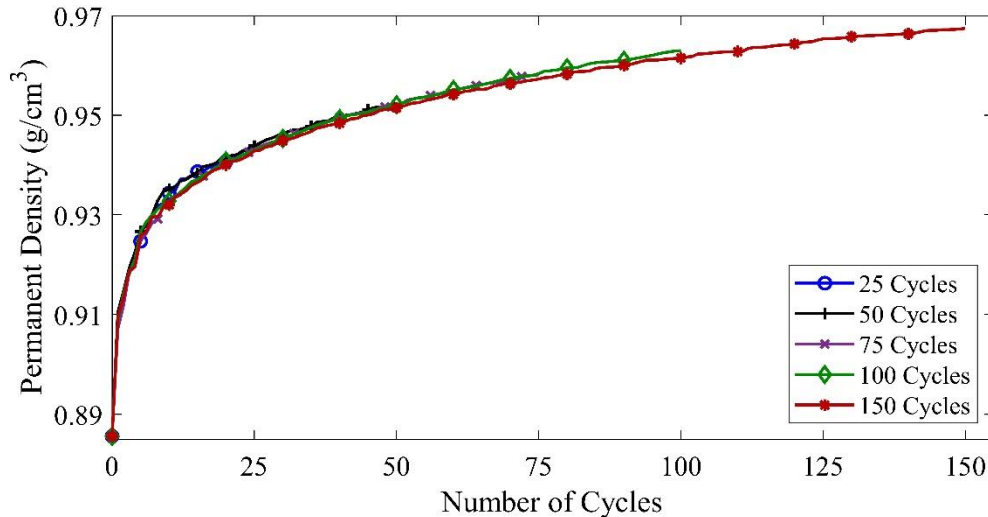


Figure 10. Effect of the number of cycles on the permanent density of the triple coke mixture (TCM) in the monotonic loading (the frequency of loading is equal to 14.79 Hz).

As shown in Figure 10, as the number of loading cycles increases, the slope of the permanent density graph decreases. As a result, in higher cycles, the amount of permanent deformation is less. This result was not far-fetched, as decreasing the distance between particles as because of increasing the density of the mixture in higher cycles reduces the amount of rotation and displacement of the particles and less permanent deformation occurs. The dependence of the anode paste density on experiments by Kansoun et al. [3] showed that the paste density is more dependent on the number of loading cycles than on the frequency. Therefore, the results of this simulation can be experimentally attributed to the behavior of coke granules in the anode paste.

4. Conclusion

In this work, the mechanical behavior of coke aggregates under monotonic and cyclic loading conditions were investigated, using the discrete element method modeling technique. The main conclusions can be summarized as follows:

- Adding small particles to the coke mixture reduces the axial pressure required for compression, thus, increasing the final density under a monotonic load and decreasing the reversible density of the mixture.
- As the rolling resistant coefficient increases, the sphericity of the particles decreases and, as a result, the compressibility of the coke mixture during the monotonic loading decreases. Hence, it causes both the maximum density and the permanent density to decrease.
- The results of the DEM simulation make it clear that in the monotonic loading on a coke mixture, the loading speed does not have much effect on the permanent density of the sample.
- The loading frequency affects the constant density of the coke mixture and increases with increasing the permanent density of the coke mixture.
- The DEM modeling of the coke mixture also makes it clear that the density of the coke mixture in the vibrocompaction process is strongly dependent on the number of process cycles, and as the number of loading cycles increases, the permanent density of the mixture also increases.

The main focus of this article is on the study of the mechanical behavior of the dry coke aggregates in the monotonic and cyclic loading. However, the carbon anode paste is very complex because it is composed of coke aggregates with very wide size distributions and also contains coal-tar pitch which acts like a viscous fluid during the compaction process. In the next step, the role of

coal-tar pitch in the vibrocompaction process of anode paste will be explored by using DEM simulation.

Acknowledgements

The authors gratefully acknowledge the financial support provided by Alcoa Corp., the Natural Sciences and Engineering Research Council of Canada and Centre Québécois de Recherche et de Développement de l'Aluminium. A part of the research presented in this article was financed by the Fonds de recherche du Québec – Nature et Technologies by the intermediary of the Aluminium Research Centre – REGAL.

References

1. W.T. Chate and Green J.A.S., *US aluminum production energy requirements: Historical perspective, theoretical limits, and new opportunities*, US Department of Energy, Energy Efficiency and Renewable Energy, Washington, DC, USA, 2003.
2. Kamran Azari et al., Influence of mixing parameters on the density and compaction behavior of carbon anodes used in aluminum production, *Advanced Materials Research, Trans. Tech. Publ.*, Vol. 409, (2012), 17-22.
3. Zahraa Kansoun et al., Compaction of cohesive granular material: application to carbon paste, *Materials*, Vol. 14, No. 4, (2021), 17 pages.
4. Kamran Azari et al., Compaction properties of carbon materials used for prebaked anodes in aluminum production plants, *Powder Technology*, Vol. 246, (2013), 650-657.
5. Stéphane Thibodeau et al., High temperature compression test to determine the anode paste mechanical properties, *Light Metals*, Springer, (2014).
6. Stéphane Thibodeau et al., New insight on the restructuring and breakage of particles during uniaxial confined compression tests on aggregates of petroleum coke, *Powder Technology*, Vol. 253, (2014), 757-768.
7. Catherine O'Sullivan, Liang Cui and Stuart C. O'Neill, Discrete element analysis of the response of granular materials during cyclic loading, *Soils Foundation*, Vol. 48, (2008), 511-530.
8. Masoud Darabi et al., A modified viscoplastic model to predict the permanent deformation of asphaltic materials under cyclic-compression loading at high temperatures, *International Journal of Plasticity*, Vol. 35, (2012), 100-134.
9. Roozbeh Mollaabbasi et al., Effect of fine coke particles on rheological properties of the binder matrix of carbon anodes in aluminium production process, *The Canadian Journal of Chemical Engineering*, (2021), 1-14.
10. Roozbeh Mollaabbasi et al., Rheological characterization of pitch and binder matrix, *Proceedings of the 36th International ICSOBA Conference*, Belem, Brazil, 2018.
11. Hicham Chaouki et al., Viscoplastic modeling of the green anode paste compaction process, *Journal of Applied Mechanics*, Vol 83, No. 2, (2016), 021002.
12. Alireza Sadeghi-Chahardeh et al., Discrete element method modeling for the failure analysis of dry mono-size coke aggregates, *Materials*, Vol. 14, No. 9, (2021), 2174.
13. Alireza Sadeghi-Chahardeh et al., Effect of particle size distributions and shapes on the failure behavior of dry coke aggregates, *Materials*, Vol. 14, No. 19, (2021), 5558.
14. Behzad Majidi et al., Packing density of irregular shape particles: DEM simulations applied to anode-grade coke aggregates, *Advanced Powder Technology*, Vol. 26, No. 4, (2015), 1256-1262.
15. Behzad Majidi et al., Discrete element method investigation of bulk density and electrical resistivity of calcined coke mixes, *Metals*, Vol. 7, No.5, 9 pages.
16. Geoffroy Rouget et al., Electrical resistivity measurement of petroleum coke powder by means of four-probe method, *Metallurgical and Materials Transactions B.*, Vol. 48, No. 5, (2017), 2543-2550.

17. Peter A. Cundall and Strack Otto D.L., A discrete numerical model for granular assemblies, *Geotechnique*, Vol. 29, No.1, (1979), 47-65.
18. Shiwei Zhao, T Matthew Evans and Xiaowen Zhou, Shear-induced anisotropy of granular materials with rolling resistance and particle shape effects, *International Journal of Solids and Structures*, Vol. 150, (2018), 268--281.
19. Rodaina Aboul Hosn et al., Discrete numerical modeling of loose soil with spherical particles and interparticle rolling friction, *Granular Matter*, Vol 19, (2017), 1-12.
20. Václav Smilauer et al., Yade Documentation, *The Yade Project*, Vol. 474, No. 1, (2010), 474 pages.
21. Kamran Azari et al., Influence of coke particle characteristics on the compaction properties of carbon paste material, *Powder Technology*, Vol. 257, (2014), 132-140.
22. Reza Naghdabadi, Mohammad Javad Ashrafi and Jamal Arghavani, Experimental and numerical investigation of pulse-shaped split Hopkinson pressure bar test, *Materials Science and Engineering: A*, Vol. 539, (2012), 285-293.