Effects and optimization of ratio of particle size grading on compaction density of calcined coke particles

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Abstract
The bulk density of the anodes affects the energy consumption and associated carbon emissions of the calcined anodes over the course of the Hall-Héroult process. The bulk density of the anode mainly depends on the compaction density of calcined coke particles. In this paper, the vibro-compacting process of calcined coke particles is simulated using discrete element method. The particle behavior during vibro-compacting process and the inter-particle contact information with different ratios of particle size grading are investigated. The effects of different ratios of particle size grading on the compaction density and microstructure are studied. The critical average diameter which can distinguish whether the compaction density meets standard requirement is first proposed and obtained. The triangular coordinate graphical is introduced to optimize the ratio of particle size grading which is different from conventional method. The results show that the larger the proportion of coarse particle and medium particle, the more large voids between particles, and the increase of fine particle can effectively fill the inter-particle gap. The critical average diameter of calcined coke particles is 2.26 mm, and average diameter less than 2.26 mm can meet the standard requirement. The optimal ratio of particle size grading is 46% for coarse particle, 12% for medium particle and 42% for fine particle.

1. Introduction
The Hall-Héroult reduction process which is used to produce aluminum is a high energy consumption process [1–3]. As a consumable material, pre-baked anode has always been the research focus of energy saving in the aluminum electrolysis industry. On the one hand, the voltage drops of anode account for about one tenth of the electrolysis voltage [4]. On the other hand, the life cycle of the anode has a remarkable influence on the aluminum electrolysis production cycle. Prolonging the life cycle can greatly reduce the anode consumption, maintain the balance of energy and material, as well as reduce the costs of anode production and transportation [5, 6]. The electrical conductivity and porosity of the anode have great impact on the carbon consumption (greenhouse gas) and the initiation and propagation of cracks in the baked anode [7]. Thus, energy-saving and cost-reducing of pre-baked anode can be achieved mainly through optimizing the production process to improve electrical conductivity and reduce air permeability [8–10].

The green anodes are made by vibro-compacting the anode paste which is made up of calcined coke aggregates and coal-tar or petroleum pitch. The physical and chemical properties of pre-baked anode, such as electrical conductivity, air permeability and air/CO₂ reactivity, are mainly dependent on the bulk density and porosity of the green anode [11, 12]. Zuca et al [13] studied the relationship between carbon anode potential and the anode porosity in aluminum electrolysis process and found that decreasing the porosity can effectively reduce the anode voltage drop. Liu et al [14, 15] found that the purity of medium particles has a great influence on the anode quality. The larger the bulk density, the lower the porosity and air/CO₂ reactivity. Therefore, increasing the anode density improves the anode quality.
Currently, more attention is being paid to investigate the influence of parameters on the compaction density and increase anode density [16–20]. Azari et al [5, 11, 21, 22] studied the effects of mixing temperature, mixing time, coke particle characteristic and particle shape on the compaction properties of anode paste. Discrete Element Method (DEM) is now widely used to simulate the behavior of granular materials in industrial applications [23]. Majidi et al [24, 25] simulated the vibration process of calcined coke particles and obtained the vibrated bulk density, which is consistent with the experimental results. Effects of different size distribution of particles on vibrated bulk density and electrical resistivity were also studied. The above research is well done, but there are still some problems to be solved. The effect of ratios of particle size grading on particle behavior, microstructure and the contact information between particles, as well as bulk density of anode is not clear. The external load during vibro-compacting process also has a great influence on the rearrangement of particles. The method to obtain the optimal ratio of particle size grading has not been solved. Thus, further research is necessary to determine how the ratio of particle size grading affects density.

The coke particles make up the skeleton for the anode, and pitch penetrate through coke pores and fill the voids between the coke particles. The pitch binds the particles together. Good interaction between coke and pitch is an essential condition for the generation of satisfactory bonding between these two components [25–27]. The bulk density of green anode mainly depends on the compaction density of calcined coke particles [28]. In addition, the results of relevant literature studies show that a part of the binder pitch is vaporized during the baking process, creating pores and shrinkage cracks. Furthermore, pitch is the most reactive part of a baked anode to air and CO2 attacks [29, 30]. Therefore, a lower pitch content is favorable for chemical reactivity and thus the service life of anodes [25]. Thus, the increasing of the compaction density not only reduces the amount of pitch but also increases the bulk density of the green anode.

In this work, in order to clarify how the ratio of particle size grading affects the compaction density and microstructure of anode, DEM is used to simulate the vibro-compacting behavior of calcined coke particles. The Hertz–Mindlin contact model is adopted to describe the contact between particles. The particle behavior during vibro-compacting process and the inter-particle contact information with different ratios of particle size grading are investigated. The effects of different ratios of particle size grading on the compaction density and microstructure of anode are compared and studied. Based on the simulations, the critical average diameter which can distinguish whether the compaction density meets standard requirement is obtained, which has not been proposed before. Triangular coordinate graph is used to obtain the optimal ratio of particle size grading for guiding production of anode, which is different from conventional method. The optimal ratio of particle size grading can be used for anode production to further improve anode quality and reduce the amount of pitch.

2. Numerical model and method

2.1. Hertz–Mindlin contact model

Contact model is an important theoretical principle of DEM, which directly determine the magnitude of force and moment of particles. For the vibro-compacting process of calcined coke particles, the inter-particle force is mainly composed of elastic force, mass force and friction force [31]. Due to the fact that calcined coke particles are unbounded and small strain in the vibro-compacting process, the Hertz–Mindlin contact model is employed in the present study [32, 33].

The normal force \( F_n \) is defined as the following formula [31, 32]:

\[
F_n = \frac{4}{3} E_{eq} \sqrt{R_{eq} \delta_n^2}
\]  

(1)

where \( E_{eq}, R_{eq} \) and \( \delta_n \) are equivalent Young’s modulus, equivalent radius and normal displacement, respectively. \( E_{eq} \) and \( R_{eq} \) are defined as follows:

\[
\frac{1}{E_{eq}} = \frac{1 - \nu^2_i}{E_i} + \frac{1 - \nu^2_j}{E_j}
\]

(2)

\[
\frac{1}{R_{eq}} = \frac{1}{R_i} + \frac{1}{R_j}
\]

(3)

where \( E \) and \( \nu \) are the Young’s modulus and Poisson’s ratio, respectively. \( R \) is the distance between the contact point and the center of mass for object. The subscript \( i \) and \( j \) identify the object \( i \) and object \( j \).

The normal damping force \( F_{nd} \) is given by [31, 32]

\[
F_{nd} = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_n m_{eq}} v_n^{rel}
\]

(4)
where $\beta$ is a parameter related to the coefficient of restitution $e$, $S_n$ is the normal stiffness, $m_{eq}$ is the equivalent mass and $v_{n}^{rel}$ is the normal component of the relative velocity. These parameters can be calculated as follows:

$$\beta = \frac{\ln e}{\ln^2 e + \pi^2}$$

$$S_n = 2E_{eq}\sqrt{R_{eq}\sigma_n}$$

$$\frac{1}{m_{eq}} = \frac{1}{m_i} + \frac{1}{m_j}$$

The tangential force $F_t$ is given by the Mindlin–Deresiewicz theory [31, 34]:

$$F_t = -S_t \delta_t$$

where $\delta_t$ is the tangential displacement and $S_t$ is the tangential stiffness.

$$S_t = 8G_{eq}\sqrt{R_{eq}\delta_t}$$

where $G_{eq}$ is the equivalent shear modulus and $\delta_t$ is the tangential displacement. $G_{eq}$ is defined as

$$G_{eq} = \frac{2 - \nu_i}{G_i} + \frac{2 - \nu_j}{G_j}$$

The tangential damping force $F_{td}$ is defined as

$$F_{td} = -2\sqrt{\frac{5}{6}}\beta S_t m_{eq} v_{n}^{rel}$$

where $v_{n}^{rel}$ is the tangential component of the relative velocity. The tangential force is limited by Coulomb friction, $\mu F_n$, where $\mu$ is the coefficient of static friction.

Rolling friction, which is accounted by applying a torque to the contacting surfaces, is important for simulations.

$$\tau_i = -\mu_r F_i R_i \omega_i$$

where $\mu_r$ is the coefficient of rolling friction and $\omega_i$ is the unit angular velocity of object $i$ at the contact point.

2.2. Simulation method

2.2.1. Physical model

The vibro–compacting processes of the calcined coke particles using different ratios of particle size grading are simulated. There are three kinds of particle sizes: coarse particles ($5 \sim 15$ mm), medium particles ($1.5 \sim 5$ mm) and fine particles ($0.5 \sim 1.5$ mm). According to the principle of similarity theory, the simulation model is one-tenth of the actual size of anode, which reduces the computation load without affecting the accuracy of calculated results.

Figure 1 shows the sketch map, of which the red upper surface is the pressure load surface, black particles are the coarse particles, green particles are the medium particles, as well as the gray particles are the fine particles. In this study, the ratio of particle size grading is provided by an anode manufacturing plant. The coarse particles account for 30%, the medium particles account for 30%, the fine particles account for 40%, and all of which are stacked in the mould with the three dimensions 155 mm $\times$ 66 mm $\times$ 60 mm. Although coke particles are not spherical, they can be treated as spherical particles according to the results of dry aggregates compression test in [35]. There are 19 189 sphere particles with different diameters randomly generated by built-in particle generation command in the software.
2.2.2. Boundary conditions
The anodes are made by vibro-compacting the calcined coke particles. The vibration and compression are applied simultaneously. The sinusoidal vibration load with the amplitude of 1 mm and the frequency of 30 Hz along the Z direction is applied in vibration process. For the compression process, the load with initial compression speed $0.08 \text{ m s}^{-1}$ is exerted on the upper surface of the model. These process parameters are provided by the equipment manufacturer. According to the instructions of the equipment, the maximum load on the upper surface is 0.15 MPa. Once the load on the upper surface reaches 0.15 MPa, the calcined coke particles are completely compressed. The other surfaces are treated as fixed wall boundary condition.

2.2.3. Calculation parameters
The basic assumption of DEM is that time step should be small enough to ensure the disturbance from other non-contact elements cannot spread to particles contacting each other within one single time step. Given the great importance of time step, it is determined according to Rayleigh wave method

$$
\Delta t_c = \left[ \frac{R}{0.163 \nu + 0.877 \sqrt[3]{\frac{\rho}{G}}} \right]_{\min}
$$

where $G$ is the shear modulus, $\nu$ is the Poisson’s ratio and $\rho$ is the density of particles. Time step is calculated by equation (13) when particles are in static state or relative speed between particles is small, which can ensure the stability of the calculation system. In this study, time step is $7.28 \times 10^{-7} \text{ s}$.

The collision and friction between particles can lead to kinetic energy loss, so we need to consider the collision and friction including particle-particle and particle-wall. The collision and friction dynamics behavior is affected by material properties and motion state. The physical properties of the materials are shown in table 1. Young’s modulus and Poisson’s ratio of calcined coke particles were measured by a dynamic elastic modulus tester according to the ASTM E1876–01 standard test method. Particle density was measured by a pycnometer (Micrometrics AccuPyc1340), which is based on Archimedes principle-gas expansion replacement method. The wall material is steel, and the related physical parameters are recorded in the material library of EDEM software.

2.2.4. Model verification
In order to validate the mathematical model mentioned above, three cases with different ratios of particle size grading were numerically simulated to compare with the experimental results reported in the [37]. Table 2 shows experimental and numerical results of compaction density. It is seen from the table that the simulation and experimental results show good agreements, and the relative error is within 5%, which is acceptable. Thus, this method can effectively predict the compaction density of calcined coke particles with different ratios of particle size grading.

| Table 1. Physical properties of the calcined coke particles and steel wall. |
|-------------------------------------------------|
| Properties                                      | Value |
| Young’s modulus of particle (Gpa)               | 36.5  |
| Poisson’s ratio of particles                    | 0.425 |
| Particle density (g cm^{-3})                    | 2.46  |
| Young’s modulus of wall (Gpa)                   | 206   |
| Poisson’s ratio of wall                         | 0.3   |
| Density of wall (g cm^{-3})                     | 7.8   |

| Table 2. Comparisons between numerical results and experimental data for compaction density [37]. |
|---------------------------------------------|
| Coarse particles (%) | Medium particles (%) | Fine particles (%) | Simulations (kg m^{-3}) | Experiments (kg m^{-3}) | Error |
|---------------------|----------------------|-------------------|-------------------------|-------------------------|------|
| 30                  | 30                   | 40                | 1698.22                 | 1632                    | 4.06%|
| 23                  | 35                   | 42                | 1702.81                 | 1643                    | 3.64%|
| 32                  | 56                   | 12                | 1579.35                 | 1575                    | 0.28%|

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3. Results and discussions

3.1. Vibro-compacting process of calcined coke mixes

In this paper, the dimensionless time $T$ is used as the time scale, which is defined as the ratio of current compression time $t$ to the total compression time $t_{total}$. $t_{total}$ is the time required for the final load pressure on the upper surface reaches 0.15 MPa. The movements of particles in different periods of time in the longitudinal section are shown in figure 2. In the initial stage of the vibro-compacting process, almost all of the particles fall down by gravity, and the load surface has no obvious effect on the particles. When dimensionless time $T$ is 0.4, most of the particles have deposited at the bottom of the model, and the elastic collision occurs between part of the upper particles and the particles deposited at the bottom of the model. At the moment, elasticity is greater than gravity, thus fine particles move upward and collide with the upper load surface and then move downward. The movement repeats until the end of the forming process. At the bottom of the model, because the particles are dense and the movable space is small, the particles move in a small area under the vibration load and the contact force between particles. Besides, most particles move downward layer by layer in the vertical direction. Due to the vibro-compacting effect, a few smaller particles move quickly to fill into the voids. As figures 2(e) and (f) shown, the voids around coarse particle is filled by fine particles. Along with the vibro-compacting process, particles become dense and pores among particles reduce obviously. The figures also show that the density in the lower layer changes first and the porosity between particles decreases rapidly. When the pressure reaches the maximum pressure with 0.15 MPa, the compression is finished. The particles reach stable state and the bulk density tends to be uniform and stable.

3.2. The load pressure and potential energy

The load pressure on the upper surface and the potential energy of the particles can reflect the motion state of the particles. Figure 3 shows the load pressure on the upper surface varies with time. During the period from the initial stage of vibro-compacting process to time point A, the particles generated randomly in the upper part fall down under the action of gravity and the particles in the lower part move upward under the action of vibration, but the overall trend of the particles is downward. The falling velocity of most particles is larger than that of load surface and the load surface will only touch a small amount of particles that bounce to the load surface under the action of vibration. Thus, the load pressure is very small, almost zero. Starting from point A, more particles begin to contact with the upper surface and are compressed continuously. It can be seen in enlarged drawing in figure 2(e) that there are some large gaps which are not filled with small particles. As the gaps are filled during vibro-compacting process, the pressure drops suddenly at point B. If there are still gaps left in this collapse, it is
possible to collapse again causing pressure drop. As the particles accumulate more closely, the pressure on the upper load surface increases gradually, and the compression stops at point C where the pressure reaches the maximum pressure with 0.15 MPa.

The total potential energy of particles varying with time is shown in figure 4. As shown in figure 4, from the beginning of the vibro-compacting process to time point D, the total potential energy decreases sharply because the free fall of the particles. Then particles pile up at the bottom of the container and become denser during vibration process, the potential energy decreases slowly. Comparing the gradient variation of total potential energy between DA and AC in time period, it can be found that the gradient variation in AC time period is larger than that of in DA time period, which indicates that the compaction effect of particles is greater than that of vibration in the vibro-compacting process.

Combined with figures 3 and 4, it can be concluded that the particles first fall and deposit under gravity and then become dense under vibration. Finally, under the action of vibro-compacting, the particles rearrange and the fine particles fill the voids. The particles are in close contact, forming an arch structure that prevents further compression. As the load pressure increases, the particles first elastically deform and then slide, and the arch formed by the accumulation of particles is destroyed [28]. The particles are further compressed. When the load pressure reaches 0.15 MPa, the particles cannot move and reach equilibrium state.

![Figure 3. The load pressure on the upper surface varying with time.](image)

![Figure 4. The total potential energy of particles changes with time.](image)
Table 3. The results of cases with different ratios of particle size grading.

| Case | Coarse particle (kg) | Medium particle (kg) | Fine particle (kg) | Density (kg m$^{-3}$) | Case | Coarse particle (kg) | Medium particle (kg) | Fine particle (kg) | Density (kg m$^{-3}$) |
|------|----------------------|---------------------|-------------------|-----------------------|------|----------------------|---------------------|-------------------|-----------------------|
| 118  | 0.05                 | 0.05                | 0.40              | 1621.66               | 343  | 0.15                 | 0.20                | 0.15              | 1737.80               |
| 127  | 0.05                 | 0.10                | 0.35              | 1637.13               | 352  | 0.15                 | 0.15                | 0.25              | 1680.56               |
| 136  | 0.05                 | 0.15                | 0.30              | 1649.75               | 361  | 0.15                 | 0.30                | 0.05              | 1578.88               |
| 145  | 0.05                 | 0.20                | 0.25              | 1664.90               | 415  | 0.20                 | 0.05                | 0.25              | 1740.39               |
| 154  | 0.05                 | 0.25                | 0.20              | 1661.21               | 424  | 0.20                 | 0.10                | 0.20              | 1741.89               |
| 163  | 0.05                 | 0.30                | 0.15              | 1680.93               | 433  | 0.20                 | 0.15                | 0.15              | 1734.63               |
| 172  | 0.05                 | 0.35                | 0.10              | 1640.15               | 442  | 0.20                 | 0.20                | 0.05              | 1702.64               |
| 181  | 0.05                 | 0.40                | 0.05              | 1590.27               | 451  | 0.20                 | 0.25                | 0.05              | 1601.71               |
| 217  | 0.10                 | 0.05                | 0.35              | 1659.03               | 514  | 0.25                 | 0.05                | 0.20              | 1738.89               |
| 226  | 0.10                 | 0.10                | 0.30              | 1664.67               | 523  | 0.25                 | 0.05                | 0.10              | 1733.30               |
| 235  | 0.10                 | 0.15                | 0.25              | 1692.81               | 532  | 0.25                 | 0.15                | 0.10              | 1734.48               |
| 244  | 0.10                 | 0.20                | 0.20              | 1697.06               | 541  | 0.25                 | 0.20                | 0.05              | 1584.77               |
| 253  | 0.10                 | 0.25                | 0.15              | 1693.85               | 613  | 0.30                 | 0.05                | 0.15              | 1716.61               |
| 262  | 0.10                 | 0.30                | 0.10              | 1668.05               | 622  | 0.30                 | 0.10                | 0.10              | 1724.60               |
| 271  | 0.10                 | 0.35                | 0.05              | 1575.27               | 631  | 0.30                 | 0.15                | 0.05              | 1663.54               |
| 316  | 0.15                 | 0.05                | 0.30              | 1680.56               | 712  | 0.35                 | 0.05                | 0.10              | 1619.03               |
| 325  | 0.15                 | 0.10                | 0.25              | 1697.81               | 721  | 0.35                 | 0.10                | 0.05              | 1514.33               |
| 334  | 0.15                 | 0.15                | 0.20              | 1698.22               | 811  | 0.40                 | 0.05                | 0.05              | 1534.24               |

3.3. The effect of the ratio of particle size grading on the compaction density

3.3.1. The compaction density of different ratio of particle size grading

In order to understand the effects of different ratios of particle size grading on the compaction density, 36 groups of simulations are designed and the results are listed in table 3. For the logical meaning of the case number, take case 334 as an example, the hundreds place indicates that the coarse particles account for 30%, the tens place indicates that the medium particles account for 30%, and the ones place indicates that the fine particles account for 40%. The total mass of particles generated in the model is 0.5 kg, while the compaction densities of generated anode in different cases vary widely. It can be seen from table 3 that there are 10 cases where the ratios of the coarse particles are the same, the average diameter increases with group of small particles with the same mass, the large particle occupies a smaller volume than these small particles. But this range is large and not optimal. The maximum compaction density is about 1741.89 kg m$^{-3}$, which occurs when the ratio of coarse, medium and fine particles is 2:1:2. It can also be concluded that an appropriate increase in the proportion of coarse and fine particles and a decrease in the proportion of medium particles help to increase the compaction density.

3.3.2. The microstructure with typical particle ratio

The microstructure of low compaction density anode with typical particle ratio is shown in figure 5. Figure 5(a) is the microstructure of anode with a large proportion of coarse particles. It can be observed from the partial enlarged drawing that although the fine particles fill the gaps between the coarse or medium particles, there are a large number of inter-particle voids between the fine particles and the distance between the fine particles is far because there are not enough fine particles to fill. Figure 5(b) is the result of case 172, in which the ratio of medium particles is large and the voids become smaller than that of in figure 5(a). The particle distribution characteristic in figure 5(c) is that small particles are closely arranged and the number of large voids is significantly reduced. Due to the large proportion of fine particles, the number of small voids between fine particles increases significantly. Compared with figures 5(a)–(c), the number of voids in figure 5(d) is significantly reduced, but there are still some obvious small voids. There is room for further optimization.

In summary, the reason for the low compaction density is the existence of voids. One large particle and a group of small particles with the same mass, the large particle occupies a smaller volume than these small particles because there are voids between the small particles. However, the gap between large particles is relatively large that requires small particles to fill. Therefore, a reasonable ratio of particle size grading can ensure the reasonable arrangement of particles to reduce the voids, achieving the purpose of increasing compaction density.

3.3.3. The relationship between average diameter and compaction density

Figure 6 shows the relationship between compaction density and average diameter in 36 groups of cases. It can be seen that in the cases where the ratios of the coarse particles are the same, the average diameter increases with...
increasing the ratios of medium particles, while the compaction density increases at first and then decreases. When the average diameter is the largest, the compaction density is the smallest. According to the production standard of anode, the bulk density should be larger than 1630 kg m\(^{-3}\). It can be seen from the figure 6 that the average diameter less than 2.26 mm can meet the minimum requirements of production. Therefore, from the viewpoint of average diameter, no matter how the ratio of coarse particles, medium particles and fine particles is, the average diameter less than 2.26 mm can meet the requirement that the anode density should be larger than 1630 kg m\(^{-3}\). The critical average diameter with 2.26 mm can be used to distinguish whether the compaction density can meet the standard requirements.

3.4. The optimization and guidance for the ratio of particle size grading
The density of anode is different with varying ratio of particle size grading. In order to obtain the optimal ratio of particle size grading, the experiments and orthogonal optimization are generally used, but it is time-consuming and cost-consuming. In the present work, the triangular coordinate graphical [38–40], which is always used for geographical analysis or for phase diagram of ternary system, is introduced to optimize the ratio of particle size.
grading. 36 sets of simulation results are used to make the triangular coordinate graph as figure 7 shows, and the relationship between ratio of particle size grading and compaction density is presented more clearly.

Figure 7 shows the relationship between the ratio of particle size grading and the compaction density of calcined coke particles. In the lower left corner of the triangular coordinate graph, where the coarse particles account for 90%~100% while the medium and fine particles are less than 20%, the density is less than 1550 kg m\(^{-3}\). This is in accord with the case of figure 5(a): the more the coarse particles, the fewer small particles that fill the voids, the smaller the compaction density. With the increasing proportion of fine and medium particles, the density is rising gradually, which means the increase proportion of fine particles can effectively increase the compaction density. It can be intuitively seen from figure 7 that the compaction density in the red region is the largest and the ratios of particle size grading in this area can be used to guide industrial production. Besides, the particle size distribution in the red area is about: the coarse particle 43% ~ 50%, the medium particle 10% ~ 20% and the fine particle 37% ~ 48%. This range is smaller than the range obtained in section 3.3.1. It can be seen from the optimal range that reducing the proportion of medium particles and increasing the proportion of coarse particles and fine particles can effectively increase the compaction density of calcined coke particles and reduce the amount of pitch. Since the bulk density of green anode mainly depends on the compression density of calcined coke particles, in order to ensure the maximization of the green anode density, the ratio of particle size grading at point A (center of the red area) can be selected as the formula guide of production. The particle size distribution at point A is as follows: coarse particles account for 46%, medium particles account for 12% and fine particles account for 42%. The compaction density calculated is 1768.38 kg m\(^{-3}\), which is larger than standard requirements and the compaction density of 36 cases.

Figure 6. The relationship between average diameter and compaction density.

Figure 7. The relationship between the ratio of particle size grading and the compaction density of calcined coke particles.
To verify whether the optimal ratio of the particles size grading is practical, we conducted three groups of experiments, one of which is the optimal ratio obtained by simulation, and the other two are the ratios within the optimal range. The results are shown in table 4. It can be seen that the compaction density of the optimal ratio is larger than that of the other two, indicating that the obtained optimal ratio of the particles size grading is in accordance with the actual situation.

4. Conclusion

In this study, the discrete element method is used to simulate the vibro-compacting process of calcined coke particles. The Hertz–Mindlin contact model is adopted to describe the contact between particles. 36 sets of cases with different ratios of particle size grading are simulated, and the optimal proportion of particle size is obtained using triangular coordinate graphical. The particle behavior, inter-particle contact information during vibro-compacting process and anode microstructure are analyzed. Based on the simulation and discussions, the following conclusions can be drawn.

(1) During the vibro-compacting process, the particles first fall to the bottom and become compact under vibration. Then the particles become denser under the pressure of the load surface. The compaction density at the bottom changes first and pores among particles reduce quickly, particles at the top move downward at the same time.

(2) The high proportion of coarse and medium particles significantly reduces the compaction density, and the increase of the fine particles could reduce the large voids, but the compaction density does not always increase with the increase of the fine particles. Reducing the proportion of medium particles and increasing the proportion of coarse particles and fine particles can effectively increase the compaction density of calcined coke particles.

(3) The critical average diameter of calcined coke particles, which can distinguish whether the compaction density meets standard requirement, is 2.26 mm. The average diameter less than 2.26 mm can meet the standard requirement that the anode density should be larger than 1630 kg m$^{-3}$.

(4) According to the triangular coordinate graph, the optimal ratio of particle size grading is obtained, that is, coarse particles account for 46%, the medium particles account for 12% and the fine particles account for 42%.

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Conflicts of interest

The authors declare no conflict of interest.

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