

A Roundness Calculation Method and Physical Parameter Analysis of A Porous Medium Model

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ABSTRACT

The rounding degree of particles is an important index of particle morphology. It represents the degree of rounding of the original edges and corners of debris particles. To a certain extent, it can reflect the transportation and deposition process of debris particles and the source properties. Therefore, it is of great significance to explore the rounding law of gravel and the influencing factors of rounding degree for the study of geological sedimentary environment, source analysis and mass transfer process. Therefore, this paper proposes a rounding degree calculation algorithm for fractal porous media model particles with rounding characteristics. Through numerical simulation and theoretical analysis, combined with the geometric parameters of particle morphology, the relationship between particle roundness and area and perimeter parameters is discussed in detail. The results show that roundness is an important factor in the geometric parameters of particles. The change of roundness can significantly affect the geometric shape of particles, and then affect the size and area of particles. It is of great significance for understanding and optimizing the flow characteristics of porous media models.

KEYWORDS

Porous Medium; Particle Shape; Roundness; B-spline curve

1. INTRODUCTION

Fractal porous media widely exist in nature and engineering applications. These complex microstructures not only determine the static physical properties of natural reservoirs, but also restrict the migration path and transport capacity of fluids [1]. The analysis of microscopic geometric morphology of pore structure is also one of the most important topics in the study of particulate matter and reservoir characterization. This is because it has an important influence on the seepage, adsorption / desorption process [2-7].

Studies have shown that morphology has an important influence on the mechanical behavior, thermal conductivity, flotation performance and other physical properties of particles[8]. In order to quantitatively characterize the influence of particle shape on various physical properties, scholars have proposed a variety of shape descriptors. According to the differences in research objects and research purposes, scholars use different shape indicators to measure collective properties, and even propose different definitions and respective calculation methods for the same indicators [9], which seriously hinders the study of particle microscopic geometry. Among many shape indexes, roundness is an important structural feature of debris particles, which indicates the degree of roundness of the original edges and corners of debris particles [10,11]. To a certain extent, it can reflect the transport and deposition process of clastic particles and the nature of provenance. Therefore, it is of great

significance to explore the law of gravel roundness and the influencing factors of roundness for the study of geological sedimentary environment, provenance analysis and mass transfer process [12,13].

The calculation of roundness usually involves the quantitative description of particle morphology and surface characteristics. Wentworth [14] gave a clear definition of roundness for the first time, and pointed out that roundness is the ratio of the sharpest corner curvature radius to the half of the longest diameter. Later, Wadell [15] improved the concept of Wentworth and pointed out that roundness is the ratio of the average radius of curvature of all corners or edges in the particle to the radius of the maximum inscribed sphere. In addition, previous studies also used the deviation between the particle contour and its least square circle (LSC), minimum circumscribed circle (MCC), maximum inscribed circle (MIC), and the deviation between the minimum circumscribed circle and the maximum inscribed circle to calculate the roundness [16]. Traditional measurement methods often rely on microscopic observation and manual measurement. Although this method is intuitive, it is inefficient and susceptible to human error. With the development of computer technology and image processing technology, more and more researchers begin to explore the calculation method of roundness based on digital image processing and computer vision. Based on the accepted definition of roundness, Nie et al. [17] proposed a roundness evaluation method based on digital image processing and B-spline generation technology.

Based on the fractal Thiessen polygon model with rounding characteristics and B-spline curve theory, this paper introduces a new rounding calculation algorithm, and makes an in-depth exploration and analysis of relevant parameters. This algorithm not only improves the efficiency and accuracy of roundness calculation, but also provides a new idea and method for the study of microscopic geometry of pore structure.

2. THEORY AND METHOD

2.1. B-Spline Curve

B-spline curve adjusts the curve shape locally through connecting points on it, which are widely used in the field of computer-aided geometric design (CAGD) and computer graphics [18,19]. It can achieve the desired precision profile by using fewer key control vertices and has continuous smoothness and strong convex hull properties. The definition of B-spline curves is generally expressed as follows:

$$C(u) = \sum_{i=0}^n B_{i,k}(u)P_i \quad (1)$$

where $B_{i,k}(t)$ is the basis function with the order of p , P_0, P_1, \dots, P_n are the control points, and n is the number of control points, The basis function $B_{i,k}(t)$ can be obtained through repeatedly using the Cox-de Boor recursion equation as follows:

$$B_{i,0}(u) = \begin{cases} 1, & u_i \leq u \leq u_{i+1} \\ 0, & \text{others} \end{cases} \quad (2)$$

$$B_{i,k}(u) = \frac{u - u_i}{u_{i+k} - u_i} B_{i,k-1}(u) + \frac{u_{i+k+1} - u}{u_{i+k+1} - u_{i+1}} B_{i+1,k-1}(u) \quad (3)$$

From this equation, it can be found that the difference in recursive equation is mainly reflected in the values of u_k and u_{k+1} . Based on the values of these nodes, it can be divided into three types: uniform periodicity, open uniformity, and non-uniformity.

Control points are used to adjust the curve shape, which is similar to simple splines. Knot points are used to divide the curve into several segments. The shape of each segment can be locally controlled, i.e., changing the coordinate of one control point will only affect the shape locally to realize more

precise control of the curve [20]. Therefore, utilizing this characteristic of the B-spline curve can effectively solve the problem of rounded edges and corners.

2.2. Roundness calculation algorithm

Particle roundness is a measure used to describe the regularity and smoothness of particle shape. Initially Wadell gave a mathematical formula for calculating roundness in his definition as shown in Eq. 4, which takes into account the radius of curvature of the particle boundary and the radius of the maximum inscribed circle. In order to calculate the roundness of the particles, a series of steps need to be followed to determine these parameters and apply the Wadell formula.

$$R_d = \sum_{m=1}^{n_{corner}} r_m / (n_{corner} * R_{max}) \quad (4)$$

where n_{corner} is the number of angles, r_m is the radius of curvature of the m -th angle, R_{max} is the radius of the maximum inscribed circle.

In order to calculate the roundness of the particles, it is necessary to calculate the maximum inscribed circle radius of the particles R_{max} and the curvature radius of each angle r_m . Based on the algorithm, the maximum inscribed circle MIC (the maximum inscribed circle) of the polygon is found, and then the number of angles is determined. Determine the best fitting circle of each angle, and finally calculate the roundness according to the Wadell definition. The specific steps are as follows:

- (1) First, to find the maximum inscribed circle of particles. The maximum inscribed circle refers to the maximum circle that can be completely located inside the particle and is tangent to the particle boundary. This usually involves using an algorithm to identify the boundary of the particle and determine the circle that can best adapt to these boundaries.
- (2) After finding the maximum inscribed circle, the next step is to identify the corner part of the particle shape contour. Corner is the contour point of the top corner, which is the position where the curvature of the particle boundary changes significantly. In order to determine these points, it is necessary to determine the normal vector of each sampling point, which can be achieved by calculating the partial derivative of the B-spline curve function. Then, the maximum inscribed circle is adjusted to be tangent to the particle boundary at all sampling points. The rules for whether the sampling point can be judged as a corner point are as follows. For a specific sampling point, as shown in Fig. 1 (a), the red point in the figure is the nearest sampling point of the judged point. If it is outside the corresponding maximum inscribed circle, it is considered that the point is located in the local concave or plane part and is not considered as a corner point. If the nearest sampling point is within the corresponding maximum inscribed circle, it can be considered as a corner point as shown in Fig. 1 (b). The above steps are repeated continuously for each sampling point along the counterclockwise direction of the particle contour to determine the corner part.

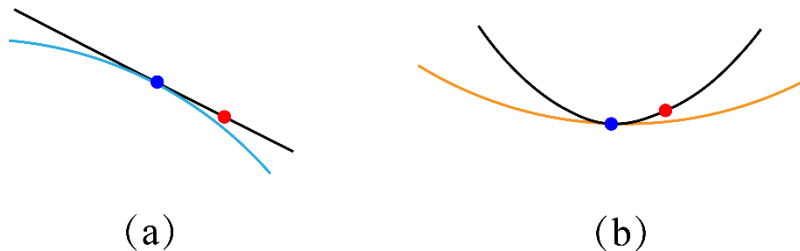


Figure 1. Determine the corner point

- (3) The radius of curvature is obtained by fitting the corner points : after all the sampling points are identified, the part of the angle can be determined by connecting the adjacent corner points. The adjacent corner points are divided into a group, and each group of corner points is identified as an angle. If there are five groups of corner points in the figure, then there are five angles. The corners of

each group are fitted with circles respectively. The gray circle in the figure is the circle of the fitted corner point. Next, the radius of curvature of each fitted circle is calculated.

In this study, the curve fitting of the diagonal points is realized by the least square method. The least squares method is a mathematical optimization technique that finds the best function matching of data by minimizing the sum of squares of errors. For the circle fitting problem, the equation of the circle and the corresponding error function are defined, where the error function represents the sum of squares of the distances from all data points to the fitting circle. The goal is to find the circle parameters that minimize the error function, that is, the center coordinates and radius.

In this paper, the optimization algorithm is used to solve the nonlinear least squares problem. Specifically, the equation of the circle and the corresponding error function are first defined, and the initial guess values of the center coordinates and radius are given. With the circular equation and error function, the optimization algorithm is used to iteratively adjust these function parameters to minimize the error function. The commonly used optimization algorithms include gradient descent method and Newton method. These algorithms determine the direction and step size of the parameter update by calculating the gradient of the error function with respect to the parameter or the Hessian matrix. In each iteration, the algorithm updates the value of the parameter according to the gradient or Hessian matrix of the current parameter and the error function, and calculates the new error function value. This process will be repeated until the convergence condition is reached (such as the error function value is less than a certain threshold, or the parameter update amplitude is less than a certain threshold). Through multiple iterations, the circle parameter that minimizes the error function is finally obtained, so as to realize the best circle fitting of the data points.

(4) Calculation of roundness : The maximum inscribed circle radius of the particle pattern extracted above and the radius of curvature of each angle identified are brought into Eq. 4, and the roundness R_d of the particle can be calculated.

In Wadell 's original roundness evaluation program, the radius of curvature (r_m) of the corner is obtained by manually fitting the circle one by one to each identified angle. This process requires manual operation, which is time-consuming and may introduce errors due to individual differences. In this paper, in order to calculate the roundness more accurately and efficiently, the algorithm function is used to automatically realize this fitting process. In this way, not only the accuracy and efficiency of roundness calculation can be greatly improved, but also the influence of human factors on the results can be reduced, making the roundness evaluation more objective and reliable.

2.3. Fractal porous media model with rounding characteristics

In this paper, a fractal porous media model based on Thiessen polygon and fractal topology theory is used, and the rounding method is applied to this model. This method constructs an inscribed circle by adding a buffer radius to the angle of the particle, thereby simulating the rounding characteristics. The following is a detailed description and analysis of this model:

The fractal porous media model in this paper creates a porous media system with complex microstructure and self-similarity through the combination of Thiessen multilateral and fractal topology theory. Thiessen polygons provide a way to divide space into multiple uniform or non-uniform regions, which are usually called Thiessen polygons or Thiessen regions. In the fractal porous media model, these polygons represent particles of different sizes and shapes.

In order to simulate the rounding phenomenon of particles in the real world, the model introduces a special algorithm, which constructs the inscribed circle by adding a buffer radius to the angle of the particles. In this way, the edges of the particles with sharp edges and corners gradually become smooth, showing the characteristics of rounding. As shown in Fig.2, the particles in the original model have different shapes and irregular boundaries. With the increase of the rounding feature (i.e., the increase of the buffer radius), as shown in Fig.2 (b), the edges of the particles begin to become

smooth, and some particles even become completely round. With the further enhancement of the roundness characteristics, the number of circular particles in the model gradually increases, and the roundness also increases. Finally, when the rounding feature reaches a certain degree, all the particles will become round, and the rounding degree reaches the maximum, as shown in Fig.2 (c). This change not only reflects the significant change of particle shape, but also reveals the influence of the rounding process on the structure and properties of porous media.

By applying this rounding method, the fractal porous media model in this paper can more accurately simulate the microstructure and properties of porous media in the real world. In addition, the model also provides us with an effective tool to study the influence of roundness on the performance of porous media, and provides new ideas and methods for future research.

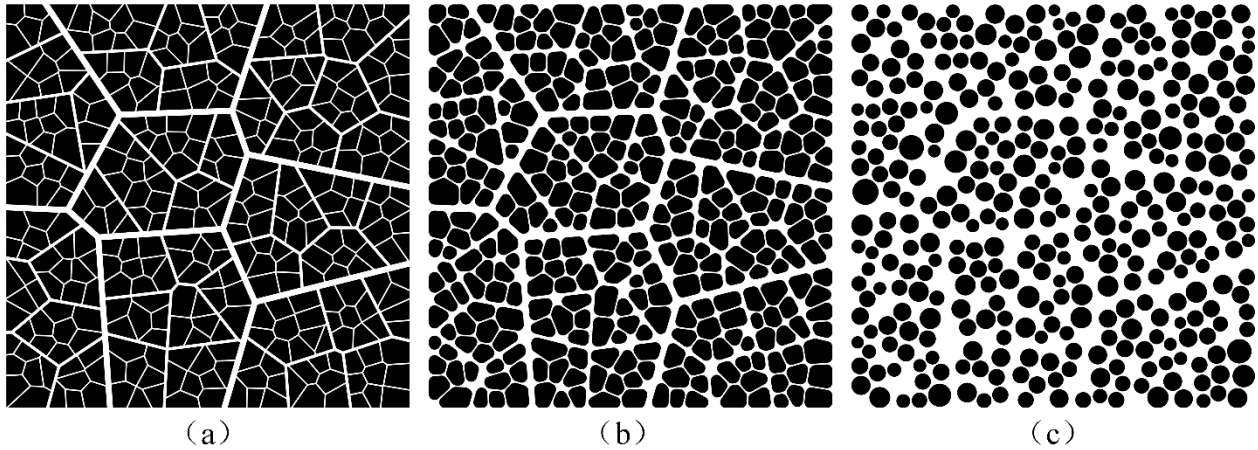


Figure 2. Porous media model with rounding characteristics

3. CONCLUSION AND DISCUSSION

3.1. The geometric feature distribution of the original model particles

Table 1. Particle area perimeter statistics of the original model

	maximum value	minimum value	mean value	variance	standard deviation
Perimeter	556.91	280.04	411.93	2837.9	53.3
Area	19275.2	4665.07	10221.97	7013535.5	2652.1

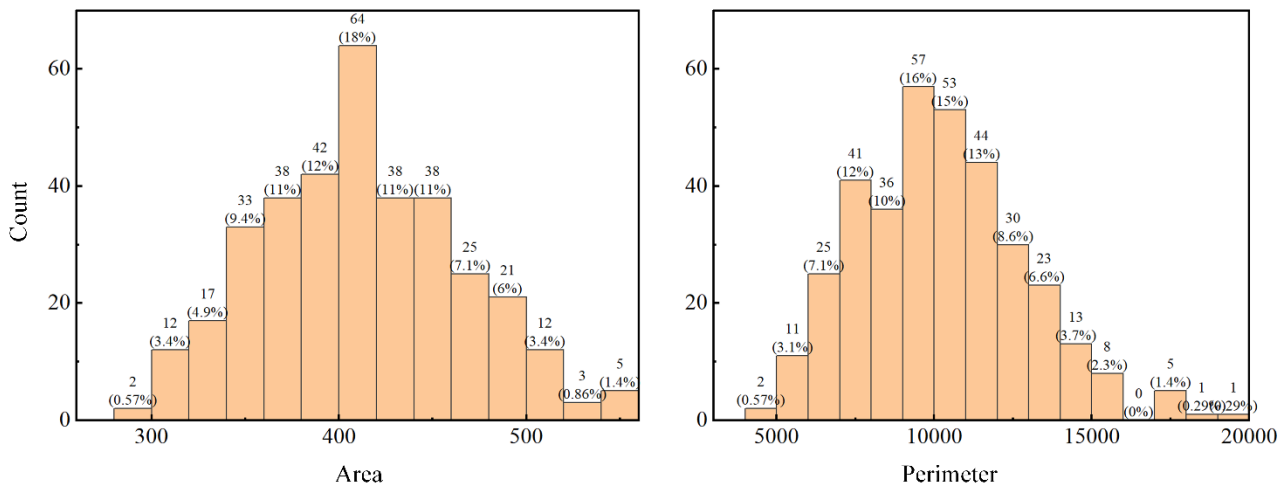


Figure 3. Particle perimeter area distribution histogram

In this paper, the area, perimeter and maximum inscribed circle of all particle polygons in the original model are calculated. Fig. 3 shows the perimeter area distribution histogram of the initial model particles. From the figure, the distribution range and proportion of all particles in the model can be observed intuitively. The maximum, minimum, average and variance standard deviation of perimeter and area are shown in Table 1.

According to the perimeter data, the maximum value is 556.91 and the minimum value is 280.04. The perimeter range of particles is relatively wide, indicating that there may be large differences in the morphology of particles. The average perimeter is 411.93, which means that the perimeter of most particles is close to this average. This is verified in the perimeter distribution histogram of Figure 3. The particles distributed between 400 and 420 account for the most, and the standard deviation is 53.3, which shows the dispersion degree of the particle perimeter distribution. Although there are some changes, the overall perimeter distribution is relatively small.

For the area data, the maximum value reaches 19275.2, and the minimum value is 4665.07. There is a significant difference between the maximum and minimum values of the particle area, which further confirms the diversity of the particles in shape and size. The average area is 10221.97, indicating that the particle area in the model is mostly concentrated at this level. However, the standard deviation is 2652.1, which is relatively high, indicating that the particle area distribution is relatively discrete and there is a large range of variation

3.2. Relationship between roundness and particle geometric parameters

Based on the established model, the selected four particles as samples, they have different initial shapes and sizes, which can reflect the diversity of particles. By adjusting the roundness coefficient, the model of the whole grinding process is obtained, and the circumference and area of these particle samples under different roundness degrees are calculated. The algorithm described above is used to calculate the roundness of these particles in the whole grinding process. The calculated data are drawn into an intuitive fitting diagram, which can deeply analyze the influence of roundness on the two key geometric attributes of particle circumference and area. At the same time, we will also observe the differences caused by different roundness coefficients on the same geometric properties, so as to understand the change law of particle morphology more comprehensively.

Fig. 4 shows the relationship between the roundness of these four particles and the perimeter and area. After observation and analysis, it is found that although these four particles are different in shape and size, their perimeter and area show an approximate change trend with the increase of roundness R_d . Specifically, with the increase of roundness, the area and perimeter of the particles show a decreasing trend. This is because as the particle shape gradually tends to be smooth, the corner part decreases, and the boundary length of the smooth shape is relatively short, which leads to the decrease of the overall surface area and perimeter.

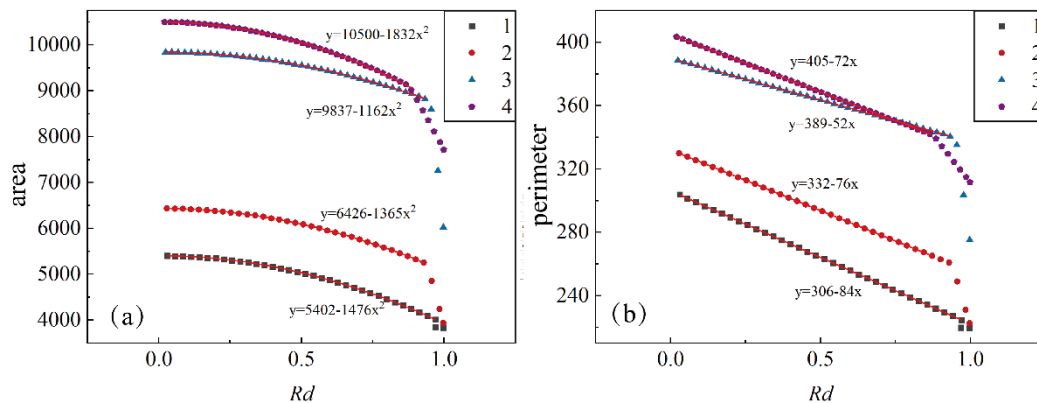


Figure 4. Relationship between roundness and particle area circumference

In further data analysis, it is found that there is a significant exponential negative correlation between particle area and roundness, that is, the higher the roundness, the smaller the area, while the relationship between perimeter and roundness is linear negative correlation, that is, the increase of roundness will lead to the linear decrease of perimeter, which is also verified by the fitting function.

It is worth noting that for particles with smaller perimeter and area, the downward trend is approximately the same, and the value of the fitting function x coefficient is relatively small. However, for larger particles, the downward trend shows obvious differences. In the case of intersection of fitting curves, the fitting functions are also quite different. The relationship between the roundness of the surface and the perimeter and area is indeed affected by the original shape and size of the particles.

4. SUMMERY

In this paper, an algorithm for calculating the roundness of fractal porous media model particles with roundness characteristics is proposed, and the rapidity and accuracy of the algorithm are verified by model application. By combining numerical simulation and theoretical analysis, the relationship between roundness and geometric parameters of particulate matter is discussed in depth, and the following important conclusions are drawn.

- 1) Roundness is one of the key factors affecting the geometric parameters of particulate matter. As the roundness increases, the original edges of the particles are gradually flattened, and the particle morphology becomes more rounded.
- 2) The change of roundness can significantly affect the geometric shape of particles. With the increase of roundness, the surface area and perimeter of the particles will change accordingly. The roundness is negatively correlated with the area and perimeter of particles. In addition, for particles with smaller perimeter and area, the downward trend is approximately the same, while for larger particles, the downward trend shows obvious differences, which indicates that the relationship between roundness and perimeter and area is indeed affected by the original shape and size of particles.

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