Mesoscopic Seepage Simulation and Analysis of Unclassified Tailings Pores Based on 3D Reconstruction Technology

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ABSTRACT: Taking the unclassified tailings as the research object, the three-dimensional (3D) pore model was established using computed tomography (CT) scanning technology, image processing, and the 3D reconstruction method. The model was imported into Flac3D software for mesoscopic seepage simulation and analysis. Combined with the laboratory seepage experiment, the influence of tailings’ mesoscopic parameters on permeability was explored. The results show that there is a high correlation between the fractal dimension and fragmentation index of tailings pores and the mesoscopic seepage coefficient, with correlation coefficients of 0.987 and 0.973, respectively. When the porosity difference of the pore model is small, the permeability is mainly affected by pore connectivity. The mathematical model between the permeability coefficient and the fragmentation index of tailings is established. The average error between the permeability coefficient calculated by the model and the measured value is reduced to 4.98%, which proves that the mathematical model has guaranteed reliability.

1. INTRODUCTION

In addition to backfilling, most of the unclassified tailings are discharged to the tailings pond for storage.1 The tailings pond is a major hazard source, prone to destabilization and dam failure under extreme conditions such as heavy rainfall.2,3 Moreover, the tailings contain a large number of heavy metal elements, which also pose a potential pollution risk to the surrounding environment.4−6 It has been studied that the permeability of tailings affects the height of the seepage line of the tailings pond, which in turn affects the stability of the dam; seepage is also the main driving force for the migration of heavy metals within the tailings. Therefore, it is necessary to study the seepage process within the pores of the tailings and the change law of the permeability properties from the mesoscopic perspective.

Unclassified tailings are unclassified and discontinuous anisotropic bodies with different types and sizes of internal pores due to differences in their original structure, which affects the permeability.7−9 At present, the determination of the permeability of tailings mainly adopts constant-head or variable-head permeability test. The research on the mesoscopic structure also mainly focuses on the description of the mesoscopic morphology of tailings. However, the macroscopic permeability determination focuses more on the variation of the overall permeability of the tailings, while neglecting the influence of the differences on the morphology of the skeletal structure of the tailing particles and the pore connectivity. It is difficult to quantitatively analyze the pore microstructure in the study of the mesoscopic structure. In recent years, the widespread application of three-dimensional (3D) reconstruction technology in the fields of materials and chemistry has made it possible to solve the above problems.

At present, foreign research in this area mainly focuses on the coupling analysis of porous media by different methods, such as 3D reconstruction and NMR, and the practice and innovation of 3D model construction principles and methods.12−17 Izadi Hossein proposed a fast and reliable 3D reconstruction method, which helped to obtain more accurate models for different sandstones;18 Yang et al. performed a detailed calculation and analysis of the porosity, pore size distribution, and connectivity of the filling mineral grain based on the self-developed Matlab 3D image analysis program;19 Lee et al. performed 3D reconstruction and micromechanical response simulation of the porous media using the Montage continuous slicing technique.20 Domestic studies have focused
on the quantitative characterization of the mesoscopic structure of tailings pores, while the interrelationship between the mesoscopic structure and permeability has been less studied.

In the study, from the perspective of the mesoscopic view, with the computed tomography (CT) scanning technology, image processing, and the 3D reconstruction method, the 3D model of tailings and pores was established, and the mesoscopic parameters were analyzed. The 3D pore model was imported into Flac3D software to simulate the mesoscopic seepage process in the pore channel of tailings. Meanwhile, combined with the laboratory seepage experiment, the

Figure 1. Mesh model of five groups of random pores.

Figure 2. Seepage process of model 1.
Therefore, the ratio of the permeability coefficient of the mesoscopic pore model is 1:1000, i.e., the permeability coefficient for each group of pore models into Flac3D and setting the model fixed pore water pressures at the nodes on the upper and lower surfaces, Pa.

The permeability coefficient \( k \) (m/s) of the pore model is calculated based on the dimensions of the model and the difference in the pore water pressure between the upper and lower surfaces of the model. The formula for the permeability coefficient \( k \) is

\[
k = \frac{Q}{L \rho g A(p_1 - p_2)}
\]

where \( Q \) is the flow rate of the pore unit on the model surface, m\(^3\)/s; \( L \) is the height of the model, m; \( A \) is the cross-sectional area of the model, m\(^2\); \( p_1 \) and \( p_2 \) are the fixed pore pressures on the upper and lower surfaces, Pa.

The permeability coefficient \( k \) is a comprehensive coefficient reflecting the water permeability of the pore and a measure of the flow rate. According to the gravity similarity criterion, the ratio of the flow rate for different-size models is \( \lambda_k = \lambda_L^{-0.5} \). Therefore, the ratio of the permeability coefficient for different-size models should be the same as \( \lambda_k = \lambda_L^{-0.5} \). The size ratio between the mesoscopic pore model and the similar experimental pore model is 1:1000, i.e., \( \lambda_L = 1 \times 10^3 \). Then, the permeability coefficient \( k_i \) of the mesoscopic model can be obtained by the following equation

\[
k_i = \frac{k}{10^{3.5}}
\]

The seepage process of the five groups of pore models is similar; therefore, model 1 is taken as an example (the grouping of “tailings” is hidden in Figure 1). From Figure 2a, it can be seen that when the water pressure in the upper surface pore is fixed at 10 MPa, water starts to percolate downward. The contour line of the pore water pressure cloud is parallel to the edge line of the top surface, indicating that there is little difference in the seepage speed around the top of the pore. Figure 2b shows that when the water has percolated 1/3 of the depth, the pore water pressure cloud becomes an arc, which is distributed along the seepage pore channel in a large to small step from top to bottom, perpendicular to the direction of the seepage velocity. From Figure 2c, we can see that the seepage depth has reached 2/3, the isolated pore channels in the \( x-z \) plane cannot be penetrated by water, and the pore water pressure remains at zero, while the water pressure in the other pore channels gradually increases as the seepage progresses. At the same height, the pore water pressure of impervious channels is higher than that of permeable channels due to head loss caused by percolation in the permeable channel, which is less than the pore pressure of the impervious passage of the same height. From Figure 2d, we can see that at this time, the flow rate of the inflow source at the top of the model is basically no longer changing, and almost all of the permeable channels are in the saturated state, which has reached a stable percolation state (Figure 1).

### 2. RESULTS AND DISCUSSION

#### 2.1. Pore Seepage Process Analysis

After importing five groups of pore models into Flac3D and setting the model length in mm, the original model was expanded by 1000 times to perform a mesoscopic seepage similarity simulation. The fixed pore water pressures at the nodes on the upper and lower surfaces of the model were \( p_1 = 10 \) MPa and \( p_2 = 0.1 \) MPa, respectively, as the inflow and outflow sources of the model. The flow rate \( Q \) of the inflow source pore unit on the upper surface of the model was recorded. It will approach a constant value when the seepage equilibrium is reached. The flow rate \( Q \) is the flow rate of the pore unit on the model surface, \( m^3/s \); \( A \) is the cross-sectional area of the object, \( m^2 \); \( p_1 \) and \( p_2 \) are the fixed pore pressures on the upper and lower surfaces, Pa.

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\]

#### 2.2. Influence of Mesoscopic Parameters on Seepage

The three-dimensional fractal dimension is a number greater than 2 and less than 3, reflecting the effectiveness of the space occupied by the complex form. It is a measure of the irregularity of the complex form, and in this case, it characterizes the degree of pore complexity. The fractal dimension \( d \) is calculated as follows

\[d = \lim_{\epsilon \to 0} \frac{\log N(\epsilon)}{\log (1/\epsilon)}\]

where \( \epsilon \) is the edge length of the cube and \( N(\epsilon) \) is the number of times the cube is used to cover the measured object.

The fragmentation index is an index that calculates the relative convexity or concavity of a surface. When considering connectivity, concavity indicates a connected structure, while convexity indicates an isolated disconnected structure, where pore connectivity is characterized. The fragmentation index \( N_i \) can be calculated by the following equation

\[N_i = \left( \frac{P_b - P_a}{A_b - A_a} \right)\]

where \( P \) and \( A \) are the perimeter and area of the object, respectively, and subscripts \( a \) and \( b \) indicate before and after image expansion.

After the software calculation, the porosity, fractal dimension, fragmentation index, and mesoscopic permeability coefficient \( k_i \) for each model are shown in Table 1. The model 3’s pore volume ratio of 62.5% is the maximum among the five groups of models, and its permeability coefficient of \( 7.336 \times 10^{-6} \) cm/s is also the maximum. This is consistent with the general rule that the permeability coefficient increases with the increase of the porosity of the porous medium because a larger porosity makes it easier for water to flow through. However, when the difference in porosity is small, such as when comparing models 1 and 5 and models 2 and 4, the model with greater porosity has a lower permeability coefficient. The reason is that the pores do not all constitute seepage channels, e.g., the isolated pore in the \( x-z \) plane in Figure 6d is not
connected to other pores, so the region is less connected and less permeable.32–34

The linear relationship between the fragmentation index and the permeability coefficient is evident from Table 2, and the fit with the linear regression equation (Formula 5) and the correlation coefficient $R^2$ of 0.987 is shown in Figure 3a. The fractal dimension and the permeability coefficient of the parameters have an obvious negative correlation, and the fit with the regression equation (Formula 6) (the defined domain is a decreasing interval) and the correlation coefficient $R^2$ of 0.973 is shown in Figure 3b. From Figure 3, we can see that the permeability of pores increases with pore connectivity and decreases with pore complexity. To a certain extent, the fractal dimension can reflect the pore connectivity, that is, the fragmentation index, and there is a clear correlation between them.

$$k_i = 1.535N_i \times 10^{-4} + 9.198 \times 10^{-6}$$ (5)

$$k_j = -0.0025d^2 + 0.0118d - 0.014$$ (6)

When there is a big difference in porosity, the permeability of the larger porosity model tends to be better because the larger pores are more likely to allow water to percolate. However, when the difference in porosity is small, porosity is no longer the dominant factor affecting the permeability, while the effect of pore connectivity on seepage is more pronounced.35–38

### 2.3. Mathematical Modeling of the Permeability Coefficient

The permeability coefficient of unclassified tailings is tested using a TST-55 permeameter. According to Darcy’s law, the permeability coefficient at $T (^\circ C)$ can be expressed by the following equation

$$k_T = \frac{QL}{A\Delta h t}$$ (7)

where $Q$ is the percolation volume, cm$^3$; $L$ is the percolation height, cm; $\Delta h$ is the head loss, cm; $A$ is the cross-flow cross-sectional area, cm$^2$; and $t$ is the percolation time, s.

As shown in Table 2, the mean value of the laboratory test of the tailings permeability coefficient at a water temperature of 20 $^\circ C$ is $1.204 \times 10^{-5}$ cm/s.

From the comparison of Tables 1 and 2, we can see that the permeability coefficient calculated by the numerical simulation experiment is much smaller than the laboratory test value. This is because the permeability coefficient measured by the numerical simulation ignores the mechanical coupling of the seepage process to ensure that the structure of the tailings samples remains unchanged, which has errors with the actual situation.39

Dividing formula 1 and formula 5, we can get

$$k = \frac{QL}{A(p_1 - p_2)(1.535N_i \times 10^{-4} + 9.198 \times 10^{-6})}$$ (8)

Substituting formula 2 into formula 8, we can get

![Figure 3. Fitting results of the mesoscopic parameters and the permeability coefficient of the model.](https://doi.org/10.1021/acs.omega.1c01092)
## 3. CONCLUSIONS

Permeability is one of the important physical properties of tailings in the tailings pond. The stability of tailings pond, migration, and diffusion of heavy metals and other harmful pollutants in tailings are closely related to the permeability of tailings particles. In the paper, from the perspective of mesoscopic view, a combination of 3D reconstruction and numerical simulation is used to analyze the mesoscopic seepage process of tailings pores and the influence of mesoscopic parameters of tailings on permeability performance. The specific conclusions are as follows.

Using 3D reconstruction technology and a watershed algorithm to establish and partition the pore model of tailings with high precision, the pore volume percentage calculated by Avizo software is 48.32%, which shows a very small difference from the measured porosity of the tailings sample of 47.62%, proving that the 3D reconstruction model of tailings pores has high reliability.

Pore models with different spatial locations are imported into Flac3D for mesoscopic seepage simulation analysis. When the difference of porosity is large, the model with larger porosity has better permeability, which is consistent with the general rule that the permeability coefficient increases with the increase of porosity of porous media. When the difference of porosity is small, the model with larger porosity has a smaller permeability coefficient. The reason for this is that porosity is no longer the main factor affecting permeability. However, the influence of the pore connectivity on permeability is more significant. The fragmentation index characterizing the pore connectivity and the fractal dimension characterizing the pore complexity were calculated and analyzed for their correlation with the pores mesoscopic permeability coefficient as follows: the permeability coefficient of the pores models increased linearly with the increase of the fragmentation index and decreased significantly with the increase of the fractal dimension, and their correlation coefficients $R^2$ were 0.987 and 0.973, respectively.

Based on the results of mesoscopic seepage simulation and laboratory permeability experiments, the mathematical model between the fragmentation index and the permeability coefficient was established, which reduced the calculation error of the permeability coefficient to within 11% and revealed the variation law of the permeability performance of the tailings from the mesoscopic perspective.

## 4. MATERIALS AND METHODS

### 4.1. Sample Source and Basic Properties.

The unclassified tailings sample was taken from Sanshando Gold Mine in Shandong province, with a density of 2.73 g/cm$^3$ and a porosity of 47.62% as measured by the laboratory. The composition of tailings was determined by X-ray fluorescence spectroscopy, and the content of each element is shown in Table 4, whose chemical composition mainly includes SiO$_2$ and Al$_2$O$_3$, in addition to the presence of heavy metal elements such as Mn, Pb, Cd, and As. The particle size composition of the tailings was determined by a laser particle sizer, and its cumulative size distribution curve of the tailings is shown in Figure 4, $d_{50} = 3.53 \mu m$, $d_{10} = 18.7 \mu m$, and $d_{90} = 37.93 \mu m$, with an inhomogeneity coefficient of 10.75. The tailings are well graded.

### Table 3. Error Calculation between the Permeability Coefficient of the Mathematical Model and the Laboratory Test Value

| model number | flow (m$^3$/s) | fragmentation index | permeability coefficient $k_m$ (cm/s) | mean lab test values (cm/s) | error (%) | average error (%) |
|--------------|----------------|---------------------|---------------------------------------|-----------------------------|-----------|-------------------|
| 1            | $1.25 \times 10^{-4}$ | $-0.0339$ | $1.210 \times 10^{-5}$ | $1.174 \times 10^{-5}$ | 3.07 | 4.98 |
| 2            | $4.71 \times 10^{-5}$ | $-0.0483$ | $1.020 \times 10^{-5}$ | $1.102 \times 10^{-5}$ | 13.12 | - |
| 3            | $2.22 \times 10^{-4}$ | $-0.0110$ | $1.145 \times 10^{-5}$ | $1.170 \times 10^{-5}$ | 2.64 | - |
| 4            | $1.06 \times 10^{-4}$ | $-0.0371$ | $1.241 \times 10^{-5}$ | $1.241 \times 10^{-5}$ | 3.71 | - |
| 5            | $1.41 \times 10^{-4}$ | $-0.0313$ | $1.210 \times 10^{-5}$ | $1.174 \times 10^{-5}$ | 3.07 | 4.98 |

### Table 4. Main Chemical Composition and the Content of Unclassified Tailings

|   | analytical composition (* in units of $10^{-6}$, except * for %) |
|---|---------------------------------------------------------------|
| Au$^+$ | Ag$^+$ | S | SiO$_2$ | Fe$_2$O$_3$ | Al$_2$O$_3$ | FeO | CaO | MgO | P$_2$O$_5$ | TiO$_2$ |
| 0.03 | 0.95 | 1.12 | 58.30 | 3.05 | 13.45 | 1.09 | 3.10 | 1.07 | 0.05 | 0.26 |
| K$_2$O | Na$_2$O | As | Hg$^*$ | Pb | Zn | Cd | Cr$^*$ | Mn | Cu | burning loss |
| 5.36 | 0.17 | 0.008 | 0.11 | 0.006 | 0.015 | 0.004 | 4 | 0.09 | 0.005 | 4.17 |
4.2. CT Scan and 3D Reconstruction of Tailings. First, 30 g of dried unclassified tailings sample was put into a 10 mL centrifuge tube, and a gauze was inserted to compact the tailings to ensure that the tailings would not move during the test. The centrifuge tube was placed in a Zeiss MicroXCT-400 micro-CT test chamber as shown in Figure 5 (Photograph courtesy of Gao Yuan, Institute of Physics, Chinese Academy of Sciences. Copyright 2021. Image is a free domain). And 990 grayscale images of different height sequences were obtained after tomographic scanning of selected areas of the tailings. The image resolution was 992 pixels × 1012 pixels, and the distance between pixels was 3.4 μm. The images were cut by Avizo, and the center 400 pixels × 400 pixels square area was taken. The original CT image has problems such as noise and the difference in the scanning intensity of different tomograms, which will increase the accuracy of particle and pore recognition, thereby increasing the data error. Therefore, a series of processing on the original CT image is required: filter noise reduction—threshold segmentation—recognition of particles and pores. The binary map of the pores could be obtained by selecting 400 segmenting CT images for image preprocessing as shown in Figure 6.[40,41]

The watershed algorithm is a mathematical morphological segmentation method based on topological theory, which converts image grayscale values into gradient images and divides the image into different connected regions according to the gradient. It is widely used in the field of image processing.[42,43] The three-dimensional model of the pores can be obtained by segmenting the binary pore map with high precision using the watershed algorithm. As shown in Figure 7, the model is a cube with a side length of 1360 μm, and the pore volume accounts for 48.32% by Avizo software analysis module, which differs very little from the measured porosity of 47.62% in the tailings sample, proving the high reliability of the three-dimensional reconstructed tailings pore model.

Figure 4. Grain size composition distribution curve of unclassified tailings.

Figure 5. Zeiss MicroXCT-400 micro-CT.

Figure 6. Image preprocessing process.

Figure 7. 3D reconstruction model of pores.
4.3. Simulation Modeling of Pore Seepage in Tailings. It is necessary to establish a mesoscopic pore model for the numerical simulation of pore seepage, and the specific steps are as follows: (1) In the pore 3D reconstruction model, five groups of pore models were randomly intercepted in different spatial locations, as shown in Figure 4, and the green intercept box was the pore model used for numerical simulation experiments. (2) The advanced surface generation and meshing function of Avizo were used to manipulate the pore model, whose length × width × height was 170 μm × 170 μm × 299 μm, and it was divided into the “pore” group and the “tails” group. The pore model was imported into Flac3D software as shown in Figure 5. (3) When using FLAC3D software for seepage analysis, tailings were set as impermeable cells, i.e., model fl_null, and pores were set as isotropic permeable cells, i.e., model fl_iso. In the simulation, mechanical coupling was not performed to ensure that the structure of the tailings skeleton remains unchanged under ideal conditions.

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Notes
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