Numerical study on 3D water-air two-phase seepage characteristics of undisturbed granite residual soil at REV scale

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Abstract: To reveal the dynamic seepage mechanism of water-gas two-phase in soil, the undisturbed granite residual soil in Fuzhou was selected as the research object. Based on the computer tomography(CT) image and AVIZO-COMSOL interactive docking technology, the Level Set method was used to study the 3D water-gas two-phase seepage characteristics of the undisturbed granite residual soil at the REV scale. The results show that the residual gas in the pores is mainly distributed in blocks on the pore edges, dead corners and sudden changes of pore throats. Among the numerous pores of the REV model, there are only a few major seepage pores, which are generally characterized by wide and straight pores. In different seepage stages, the velocity distribution is different. In general, the flow velocity increases first, then decreases, and then gradually increases. The maximum velocity growth rate and decrease rate are 61.04% and 40.60%. With the increase of seepage time, the saturation of the water phase shows a sharp upward trend, and the saturation of the gas phase shows a sharp downward trend, they both occur in the initial stage of seepage, and then gradually tend to be stable. Finally, the saturation of the water phase and the residual gas phase tend to 91.86% and 8.14% respectively.

1. Introduction
Granite residual soil widely exists in the southeast coastal area of China and it is a three-phase body. It not only has solid phase (soil matrix) and liquid phase (water solution), but also has gas phase (air). In recent years, some numerical simulation methods of seepage flow under the REV scale have been developed rapidly. Among them, the numerical simulation methods of multiphase flow mainly include: volume of fluid (VOF), phase field (PFM), lattice Boltzmann (LBM) and other methods. (1) Based on the VOF method, Luo Shujing (et al.)[1] simulated the three-dimensional turbulent flow field of the wide tail pier, and completed the correct simulation of the turbulence characteristics of the flow field. (2) Based on the PFM method, Feng Qihong (et al.)[2] constructed a three-dimensional pore structure model of sandstone reservoirs, and studied the effects of its displacement rate, fluid properties, and wettability on the distribution of remaining oil and the degree of recovery. (3) Based on the LBM method, Zakirov (et al.)[3] studied the disorder of porous media in the process of two-phase drainage and its coupling with flow velocity, viscosity ratio, and surface tension on the dynamics of interface development. The above-mentioned related studies have achieved fruitful results, but they are mostly focused on the study of multiphase flow in rocks, coal seams, etc., and the PFM method requires high-precision resolution to solve the accuracy of the two-phase interface, which will seriously affect the time step selection. The LBM method has a huge demand for the computing power of the computer, especially the complicated real 3D pore model has a long computing time. The Level Set method is
first proposed by Osher and Sethian [4]. Scholars at home and abroad have applied it to the field of numerical simulation of two-phase flow [5]. However, due to quantitative technology, regional differences and other reasons, it is mostly concentrated in the plane 2D pore structure model, and there is little research on the migration process of real three-dimensional pore two-phase seepage in REV scale granite residual soil.

In view of this, this paper selects the undisturbed granite residual soil as the research object, performs industrial CT scanning on it and establishes a REV model that truly reflects the pore structure of the soil. Based on the AVIZO-COMSOL interactive docking technology, the Level Set method is used for numerical simulation to visually show the dynamic process and velocity field distribution of the water and gas two-phase seepage in the soil pores, and analyze the changes in water and gas saturation at different time steps. The research results can provide a research method and theoretical basis for further understanding the pore seepage law of granite residual soil.

2. Samples and methods

2.1 Sampling and CT scan test
The undisturbed soil of the test was selected from a slope in northwest Fuzhou. The field sampling is shown in Figure 1. The dense vegetation was selected. Before sampling, the surface humus layer was cleaned with a spade. The cleaning area was 100cm×100cm, and the thickness was 20cm. Finally, the soil column sample with the size of 15cm×15cm×40cm was obtained, and the basic physical parameters of the soil sample were tested. The results are shown in Table 1.

![Fig.1 Sampling of undisturbed soil](image)

| Table 1 Basic physical parameters of the selected sample |
|--------------------------------------------------------|
| Natural density $\rho$/ (kg·m$^{-3}$) | Moisture content $\omega$/ % | Void ratio | Liquid limit $\omega_L$/ % | Plastic limit $\omega_P$/ % | Permeability/μm$^2$ |
| 1981 | 18.42 | 0.722 | 34.82 | 20.18 | 0.446 |

The obtained undisturbed soil samples were scanned by industrial CT, the equipment name is C450KV high energy industrial CT, the working voltage is 450kV, the current is 63mA, and the lowest resolution is 150μm. The soil column sample was dried before scanning, and then the sample was scanned by cone beam. The imaging time was 500ms. The conventional start-stop scanning mode was used, and the sample was then cut into 2600 horizontal layers. The slice thickness of each horizontal layer was 0.15mm. A typical section of the sample is shown in Figure 2.
2.2 REV Selection and 3D Reconstruction

Before performing three-dimensional reconstruction of the image, the threshold value of the sample is 19920 by using the fitting method \cite{6}, Figure 3 shows the threshold segmentation map of the 3D image section (depth 8cm, 16cm, 24cm, 32cm) of the sample after noise reduction using the median filter. The blue is the pore area and the gray is the matrix area.

On the basis of the representative volume unit (REV) selection method of Ni (et al.) \cite{7}, this paper uses the 3D reconstruction model of the original size of the sample and increases the size from the center point to the surrounding area to obtain the REV corresponding to Figure 4(a). Analyzing the relationship between REV size and porosity, the results are shown in Figure 4(b). It can be found from the figure that the REV porosity hardly changes when the sample unit size is larger than 300 voxels, so the REV of 300×300×300 voxels is finally selected as the object of subsequent study on the water-gas two-phase seepage characteristics of the undisturbed soil, which will ensure the smoothness of AVIZO-COMSOL interactive docking numerical simulation.

The 3D reconstruction of undisturbed soil and the construction of connected pore model can be realized by AVIZO software. Using the AVIZO threshold segmentation function, the selected REV of the sample is subjected to 3D reconstruction. Based on the three-dimensional reconstruction model, the pore connectivity test is performed to delete isolated and unconnected pores to obtain a 3D connected pore model of the undisturbed soil. The result is shown in Figure 5(a), and the actual size is 4.5×4.5×4.5cm.
2.3 AVIZO-COMSOL interactive docking
AVIZO software's operations such as model simplification, mesh division, mesh optimization and repair, and mesh testing is used to obtain high-quality 3D connected pore models, and output STL model file that can be interactively docked with the multi-physics coupling finite element software COMSOL is output, which provides a good foundation for subsequent simulations, as shown in Figure 5(a)(b)(c). At this point, the visualization data connection process between COMSOL and AVIZO 3D model is completed. Otherwise, the above steps need to be repeated to re-divide the mesh.

\begin{align}
\rho(u\nabla)u &= \nabla \left( -pI + \mu \left( \nabla u + (\nabla u)^T \right) \right) + \rho g + F \\
\rho \nabla \cdot u &= 0
\end{align}

In the formula: \( \rho \) is the fluid density, kg⋅m\(^{-3}\); \( p \) is the pressure, Pa; \( I \) is the unit matrix; \( \mu \) is the hydrodynamic viscosity, Pa⋅s; \( F \) is the volume force, N⋅m\(^{-3}\); \( g \) is the acceleration due to gravity, m⋅s\(^{-2}\).

The interfacial tension \( \mathbf{F}_\text{int} \) is defined by the following formula:

\begin{equation}
\mathbf{F}_\text{int} = \nabla \cdot \mathbf{T}
\end{equation}

\begin{equation}
\mathbf{T} = \kappa \left( I + (-n n^T) \right) \delta
\end{equation}

In the formula: \( \kappa \) is the surface tension coefficient; \( n \) is the normal vector of the interface unit, and the calculation formula is as follows:

\begin{equation}
n = \frac{\nabla \phi}{|\nabla \phi|}
\end{equation}
\( \delta \) is the Dirac function, it can be expressed by the following formula:

\[
\delta = \delta(\Phi(1-\Phi) \| \nabla \Phi) \tag{5}
\]

In the formula: \( \Phi \) is the contour of the water-gas two-phase interface.

The "Level Set" interface determines the fluid interface by tracing the contour of the level set function and the contour \( \Phi = 0.5 \) determines the position of the interface. The equation that controls the transfer and reinitialization of \( \Phi \) is as follows:

\[
\frac{\partial \Phi}{\partial t} + u \cdot \nabla \Phi = \gamma \nabla \cdot \left( \nabla \Phi - \Phi (1-\Phi) \frac{\nabla \Phi}{\| \nabla \Phi \|} \right) \tag{6}
\]

In the formula: \( \gamma \), \( \varepsilon \) is the reinitialization parameter, \( m \cdot s^{-1} \) and \( m \). In order to make the calculation of the Level Set equation more stable, usually use \( \varepsilon = \frac{h_i}{2} \), where \( h_i \) is the grid size of the interface area, and \( \gamma \) is the maximum speed that appears in the model.

Since the level set function is a smooth step function, the global density and dynamic viscosity can be determined by the following formula:

\[
\rho = \rho_w + (\rho_g - \rho_w) \Phi \\
\mu = \mu_w + (\mu_g - \mu_w) \Phi \tag{7}
\]

In the formula: \( \rho_w \), \( \mu_w \), \( \rho_g \) and \( \mu_g \) are the constant density and viscosity of water and gas.

Water is used as the displacing phase and air is the displacing phase. The specific material properties are shown in Table 2. The interfacial tension is set in reference [9].

| Table 2 Material properties |
|-----------------------------|
| category | Interfacial tension/(N·m\(^{-1}\)) | density/(kg·m\(^{-3}\)) | dynamic viscosity/(Pa·s) |
|----------|-----------------------------------|-------------------------|--------------------------|
| water phase | 4.80×10\(^2\) | 1000 | 1.01×10\(^{-4}\) |
| gas phase | 1.209 | 1.79×10\(^{-5}\) |

The simulation of two-phase flow in the pores of the soil, and the boundary conditions are set as follows: the pores of the model are filled with air at the beginning of the model. In order to make the simulation results closer to the actual situation, the pore seepage direction in the soil is set to be along the depth direction of the soil. The model is set to infiltrate at an initial pressure of 1.1kPa and flow out at 0.1kPa to ensure that the fluid flows in the pores of the soil in a laminar state, and the remaining flow boundaries and pore walls are regarded as a non-slip state.

3. Results and analysis

Figure 6(a)–(c) respectively list the dynamic distribution diagrams of the water-gas two-phase seepage process at different times, in which the green is the gas phase and the blue is the liquid phase. It can be seen from Figure 6 that as the seepage time increases, the proportion of the water phase in the pores of the soil gradually increases, while the proportion of the gas phase gradually decreases. According to the simulation results of water-gas two-phase flow, it can be clearly seen that gas phase still exists in the pores after the end of seepage, as shown in Figure 6(c). Residual gas in the pores is mainly distributed in blocks at the edges of the pores, dead corners and sudden changes of pore throats in the model. The main reason for the analysis is that the incompressible nature of the water phase prevents the water phase from invading.

In Figure 6(b), the larger pore area at the exit of the REV model channel is marked with a red ellipse. It can be seen from the figure that the water and gas two phases enter from the inlet end, and will preferentially follow the straight pore channels with larger pores to the outlet end. Compared with other pore channels, the preferential flow effect of large pores is more significant.
Figs. 6 Dynamic schematic diagram of water-gas two-phase seepage process

Figure 7(a)–(f) respectively list the velocity field distribution diagrams of the water-gas two-phase seepage process at different times, in which the red arrow is the seepage direction. It can be seen from Figure 7 that there are only a few major seepage channels in the numerous pores of the REV model, which are generally characterized by wide and straight channels. In the early stage of seepage ($t=2 \times 10^{-5} - 2 \times 10^{-4}$ s), the flow velocity distribution is relatively scattered, and the local velocity is relatively high, mostly concentrated in the narrow areas or intersections of the pores; In the middle of seepage ($t=2 \times 10^{-4} - 5 \times 10^{-4}$ s), especially near the exit, the velocity distribution is relatively uniform, but the maximum velocity of the model has a decreasing trend. In the late stage of seepage ($t=5 \times 10^{-4} - 3 \times 10^{-3}$ s), the velocity distribution becomes dispersed compared with the middle stage, and the maximum velocity increases. For example, when $t=2 \times 10^{-5}$ s, $1 \times 10^{-4}$ s, $2 \times 10^{-4}$ s, $3 \times 10^{-4}$ s, $5 \times 10^{-4}$ s and $3 \times 10^{-3}$ s, the maximum flow velocity is respectively 1.87 m/s, 4.8 m/s, 5.46 m/s, 4.31 m/s, 2.56 m/s and 4.43 m/s, indicating that as the seepage time increases, the flow velocity first increases, then decreases and then gradually increases. The reason for the analysis is that the velocity of the water-gas two-phase seepage process is controlled by the tortuous degree of the pores, and the fluid preferentially selects the main channel for seepage, there is an obvious "advantage channel", and then other narrower and tortuous pores are selected for seepage, and eventually become stable. The maximum rate of increase and decrease of speed are 61.04% and 40.60%, respectively.
In order to obtain the changes of water and gas saturation in the process of soil pore water and gas two-phase seepage, the relationship between water and gas saturation and seepage time in the model is calculated, as shown in Figure 8. It can be seen from the figure that as the two-phase seepage time increases, the water phase saturation shows a sharp upward trend, or the gas phase saturation shows a sharp downward trend, and both occur in the initial stage of seepage, and then gradually become stable. The saturation of the water phase tends to 91.86%, and the saturation of the residual gas phase is 8.14%. At the same time, it is also found that the total saturation of the water phase and the gas phase in the model is constant over time, and both are equal to 1, which conforms to the law of conservation of mass and also verifies the correctness of the numerical model [10].

4. Conclusion

(1) After the end of seepage, there is still gas phase in the pores, and the residual gas is mainly distributed in the pore edges, dead corners and sudden changes of pore throat in the model. Among the many pores of the REV model, there are only a few major seepage pores, which are generally characterized by wide and straight pores, and the preferential flow effect of pores is more significant.

(2) In different seepage stages, the flow velocity distribution is different. Generally, as the seepage time increases, the flow velocity first increases, then decreases and then gradually increases. Among them, the maximum rate of increase and decrease of speed are 61.04% and 40.60%, respectively.

(3) With the increase of seepage time, the saturation of the water phase shows a sharp upward trend, and the saturation of the gas phase shows a sharp downward trend, and both occurred in the initial stage of seepage, and then gradually become stable. Finally, the saturation of the water phase and the residual gas phase tend to 91.8 % and 8.14%, respectively. At the same time, the total saturation of the water phase and the gas phase in the model is constant over time, and both are equal to 1, which conforms to the law of conservation of mass and verifies the correctness of the numerical model.
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