Characteristics of Fluid Flow and Solute Transport in Multicrossed Rough Rock Fractures Based on Three-Dimensional Simulation

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Abstract: Fluid flow and solute transport in rock fractures are important for controlling pollutant migration in groundwater and radionuclide migration in nuclear waste disposal. The quantitative characterization of fluid flow and mass transport in crossed fractures is the key to defining solute transport in a fracture network. In this study, the characteristics of fluid flow and solute transport in rock fractures were investigated through experiments and simulation. The surface topography of these fractures was reconstructed using 3D laser scanning technology. The solute transport in crossed parallel planes and rough fractures with intersecting angles of 30°, 60°, 90°, 120°, and 150° was investigated under different initial conditions. Results show that the intersection angle and fluid velocity significantly affect the fluid flow pattern at the intersection. As the flow velocity and intersection angle increase, streamlines at the intersection of rough fractures are unevenly distributed. The fluid tends to seep into the dominant channel and has different directions of channeling flow at the intersection of fractures. An eddy phenomenon is observed at the intersection, indicating that the seepage behavior transforms into a non-Darcy flow. As the Peclet number (Pe) increases, solute migration and diffusion gradually decrease; however, the convection part gradually increases. Thus, the solute transport mode gradually changes into a streamline path mode at the intersection of fractures.

Keywords: Fractured rocks, Solute transport model, Peclet number, Channeling flow

1. Introduction

Fluid flow and solute transport in rock fractures are controlled by many factors. The pattern of solute transport in rock mass fractures should be explored to evaluate many underground projects, such as the treatment of groundwater pollutants, the geological storage of CO₂, and the disposal of nuclear waste. Fluid flow and solute transport in crossed fractures should also be quantitatively characterized to define solute transport in a fracture network [1, 2]. However, most studies have considered simple intersecting fractures but have not investigated complex fracture networks in detail. Therefore, the understanding of fluid flow and solute transport in multicrossing fractures should be enhanced.

As human activities further reach the underground space, studies have focused on groundwater in fractured rock masses and related issues. For example, during storage, nuclear waste can be efficiently...
sealed with dense granite; however, most rock masses contain a large number of fractures, which pose a potential leakage threat [3]. With the advancement of urbanization, the pollution of precious groundwater resources has become increasingly serious.

Pollutant migration in groundwater is a complicated process. It is a comprehensive result of physical, chemical, and biological interactions and hydrodynamic domination between polluted components and original components, rock and soil, and organisms in water. On the one hand, pollutant components transform fractures during migration, such as fracture corrosion by a corrosive fluid [4], which alters the roughness and aperture of fractures; on the other hand, changes in fracture morphology affect the state of fluid flowing in fractures [5].

Many researchers used the convection–dispersion equation (ADE) to describe solute transport in a fracture. For instance, Lapidus and Amundson [6] proposed a model similar to the ADE and provided a basis for conducting research on groundwater solute transport. Solute can be divided into a completely mixed mode and a streamline path mode in cross fractures. Wilson, Hull, and Robinson [7, 8, 9] found that the size, roughness, and intersection angle of fractures can significantly affect the mixing mode of solutes at the intersection of fractures. Zou et al. [10] qualitatively analyzed the influence of fracture roughness and Peclet number (Pe) on solute transport in three-dimensional orthogonal fractures. Li et al. [11] simulated the solute transport in three-dimensional cross fractures at different angles and examined the influence of the cross angle, roughness, and Pe of the fractures on solute transport.

However, rock mass fractures have strong heterogeneity, and network fractures include multiple cross fractures. A cross fracture consists of four branches with complex inlet and outlet conditions. Solute transport in a fracture is more anomalous than that in an ordinary pipeline flow. As such, it cannot be easily studied using conventional methods. Therefore, in this study, three-dimensional laser scanning technology is applied to obtain the geometric information of a rough fracture surface. A three-dimensional rough multicross fracture model is established in COMSOL Multiphysics and compared with parallel plate simulation in terms of the influence of cross angle and fracture geometry on solute transport.

2. Fracture intersection model

In accordance with the method recommended by the International Society for Rock Mechanics, all the samples are processed into cylindrical specimens with a diameter of 50 mm and a length of 100 mm. A Brazilian splitting experiment is conducted to obtain the artificial rough fractures (Figure 1).

![Figure 1. Arrangement of rough rock fractures: (a) Brazilian test and (b) fracture surface.](image)

A noncontact optical scanner (OKIO-B) is used to scan the fracture surface and obtain high-precision three-dimensional point cloud data of the fracture surface. The point cloud data are optimized via noise reduction and patching based on the scanning system and then imported to the Surfer software to reconstruct a three-dimensional fracture surface [12]. The reconstructed rough fracture surface is shown in Figure 2.
The fracture has dimensions of 10 mm in length, 5 mm in width, and 0.5 mm in fracture aperture. A single fracture is composed of upper and lower surfaces. The parameter surface is lifted and translated to form a single fissure, which is rotated to form a fracture system with different crossing angles. A parallel plate model is established (Figure 3) to explore the influence of the geometric morphology at the intersection on solute transport.

**Figure 2.** Reconstructed 3D rough fracture surface.

**Figure 3.** Fracture model: (a) Rough fracture model and (b) parallel plate model.

3. **Numerical simulation of flow and transport**

3.1. **Governing equation**

COMSOL Multiphysics 5.5 is used to simulate the fluid flow and solute transport in the fracture. For incompressible Newtonian fluid in the fractures, the N-S equation is generally utilized to describe the fluid flow in a fracture:

\[ \rho \mathbf{u} \cdot \nabla \mathbf{u} - \mu \nabla^2 \mathbf{u} = -\nabla P, \]

where \( \rho \) is the fluid density, kg/m\(^3\); \( \mu \) is the dynamic viscosity coefficient, Pa\(\cdot\)s; \( \mathbf{u} \) is the flow velocity, m/s; and \( P \) is the fluid pressure, Pa.

The ADE is used to describe the solute transport:

\[ \frac{\partial C}{\partial t} = -\nabla (\mathbf{u} C) + \nabla (D \cdot \nabla C), \]

where \( C \) is the concentration, mol/m\(^3\); \( t \) is the time, s; and \( D \) is the diffusion coefficient, m\(^2\)/s.

3.2. **Physical parameters and boundary conditions**

In COMSOL Multiphysics 5.5, the laminar (spf) physics interface is chosen to solve the N-S equation and obtain the velocity field and pressure field of single-phase flow based on the conservation of momentum and the continuity equation for mass conservation.
For the solute transport, the transport of diluted species (tds) physics interface is introduced to the transport of chemical substances and used to calculate the concentration field of a dilute solute in a solvent.

A fully developed flow velocity boundary is applied to ensure a steady flow at the inlet, and the outlet is set as a pressure boundary. No-slip and no-flow fractured walls are set. In solute transport, a solution with a concentration of $C = 1 \text{ mol/m}^3$ is continuously injected at a specific inlet, and the matrix is considered to be impermeable. The other boundary conditions are set to be no flux.

The parameters of the model are shown in Tables 1 and 2.

| Table 1. Model parameters. |
|-----------------------------|
| Fluid density $\rho$        | Acceleration of gravity $g$ | Dynamic viscosity coefficient $\mu$ | Diffusion coefficient $D$ | Solute concentration $c$ |
| 1000 (kg/m$^3$)             | 9.8 (m$^2$/s)                 | $1.307 \times 10^{-3}$ (Pa·s)        | $2.03 \times 10^{-9}$ (m$^2$/s) | 1 (mol/m$^3$)             |

The dimensionless coefficient Peclet number (Pe) is introduced to analyze the mixing of solutes at the intersection of fractures $^{[13]}$. Pe is the ratio of convective mass transfer ($N_{conv}$) to diffusion mass transfer ($N_{diff}$):

$$Pe = \frac{N_{conv}}{N_{diff}}$$

| Table 2. Model calculation parameters. |
|---------------------------------------|
| Pe | 0.5 | 10  | 50  | 100 | 200 | 500 |
| Velocity (m/s) | $2.03 \times 10^6$ | $4.06 \times 10^5$ | $2.03 \times 10^4$ | $4.06 \times 10^4$ | $8.12 \times 10^4$ | $2.03 \times 10^3$ |

4. Simulation results and analysis

4.1. Flow test

Seepage direction is complicated because of the large number of branches in multicrossing fractures. The following boundary conditions are set at the entrance and exit of the crossed fractures to achieve conditions similar to the actual working conditions: “Flow in the same direction” and “Flow in the opposite direction” (Figure 4). In Figure 4, fracture branches are represented by 1, 2, 3, 4, 5, and 6, and intersections are denoted by $\text{(1)}$ and $\text{(2)}$.

For steady-state laminar flow, streamlines are evenly distributed along the seepage direction in the parallel plate model (Figure 5). In the intersecting rough fracture, the seepage field has significant nonuniformity. When the flow velocity is high, the streamlines have different deviation degrees. The fluid tends to seep into the dominant channel and has different degrees of channeling flow at the fracture branches. Moreover, a significant eddy can be observed at the intersection of the fractures because the inertial force becomes non-negligible as the velocity in rough fractures increases.
Figure 4. Inlet and outlet conditions: (a) Same direction inflow conditions and (b) flow in the opposite direction.

Figure 5. Parallel plate streamlines: (a) Same inflow direction conditions and (b) flow in the opposite direction.

The seepage field in the fracture is greatly affected by the angle of intersection and the inlet and outlet conditions. Under the condition of the same inflow direction, channeling flow and eddy at the intersection are evident. The greater the crossing angle is, the more obvious the eddy phenomenon will be (Figure 6). Although channeling flow and eddy also occur under the condition of reverse water inflow, the possibility of streamline distribution turbulence in the fracture is greatly reduced. As the crossing angle increases, the eddy phenomenon is still more significant under the condition of the same inflow direction than that under the reverse direction of water inflow. Some reverse branches are affected by the opposite branches, thereby forming a hedging effect. Thus, the effective channel of seepage narrows.
Figure 6. The distribution of streamlines of fracture with different crossing angles: (a)–(e) Flow in the same direction and (f)–(j) flow in the opposite direction.

4.2. Solute concentration distribution

Pe can be used to analyze the mixing of solutes at the intersection of the fracture qualitatively. When Pe < 1, the diffusion effect exceeds the convection effect in terms of its contribution to the total mass flux. Solutes are fully mixed at the intersection and then transported to the exit. When Pe gradually increases, the convection effect is significant. Solute migration at the intersection of the fracture is converted from a completely mixed mode to a streamline path mode.[13,14]

In comparison with the parallel plate model, solutes move to the outlet along the channeling flow because of the channeling flow and eddy effects of the cross-rough fracture surface; as a result, they unevenly migrate in the fracture (Figure 7). When the inertial force cannot be ignored, the fluid has an eddy phenomenon in the depression or protrusion of the fracture, inevitably leading to the narrowing of the solute transport channel.[15]

Figure 8 shows the solute transport in the cross fracture under the reverse water inflow conditions of different Pe. Under reverse water inflow, solute transport is greatly affected by the inlet branch. In migration, some of the solutes seep through the outlet in the form of channeling flow. Most of the solutes are fully mixed in the retention area and become evenly distributed in the inlet branch fracture because of the effect of the hedging flow.
The intersection angle of the fractures controls the seepage channel at the intersection. The overlap between the intersecting fractures is larger, and the solutes mix more fully at the intersection. When the angle of intersection is large, the velocity of the fluid changes greatly at the intersection. Thus, solutes quickly move with the fluid to the corresponding outlet. However, they experience difficulty in reaching other outlets except the channeling part.

![Image of solute concentration distribution](image)

**Figure 7.** Solute concentration distribution at different angles and different Pe under the flow in the same direction.

![Image of solute concentration distribution](image)

**Figure 8.** Solute concentration distribution at different angles and different Pe under the flow in opposite directions.

5. Conclusions
In this study, a three-dimensional cross fracture model is established on the basis of real fracture surface morphology data. The fluid flow and solute transport in the fracture are investigated in terms of the influence of different crossing angles on fluid flow and solute transport. The main conclusions are as follows:

(1) As the flow velocity increases, the fluid tends to flow to the dominant channel at the branch of the fracture, and the fluid has different degrees of channeling. At the intersection of the fractures, an obvious eddy can be observed, the fluid flow state changes from a Darcy flow to a non-Darcy one. Under the flow in the same direction, the fluid is more prone to channeling and eddy. The hedging effect creates a blocked flow, and the fluid tends to produce channeling and eddy at the intersection.

(2) The mixing behavior of solutes is closely related to Pe. When Pe < 1, the solute transport in the fracture is mainly based on diffusion. As Pe increases, the diffusion part gradually decreases, and the convection part increases. At the intersection of the fractures, the solute transport mode changes to a streamlined path mode.

(3) The transport of solute in the fracture is significantly related to the fluid flow pattern at the intersection of the fracture. As the flow velocity increases, the eddy of the fluid causes the solute transport channel to narrow. Most of the solutes are fully mixed in the retention area because of the effect of the hedging flow and become evenly distributed in the inlet branch fracture.

6. References

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