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# Numerical Simulation of Mass Transfer Characteristics of Three-Dimensional Cross-Fracture Seepage

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## Abstract

**Quantitative description of the mass transfer characteristics of cross-fracture seepage is the basis for studying the characteristics of seepage mass transfer in the entire fracture network. In order to truly simulate the migration process of water flow and solute in three-dimensional cross fractures, first generate a three-dimensional cross fracture model, and then solve the Navier-Stokes equation, assuming that the solute migration satisfies Fick's law, simulate the migration of water current and solute in three-dimensional cross fracture process. Comparing the simulation results of the rough fracture model and the parallel plate model, it is found that the roughness has a significant effect on the distribution and flow state of the fluid; the geometry of the fracture surface will significantly affect the solute mixing behavior. The crossing angle of the fissures also has a greater impact on solute transport. These results indicate that the currently widely used parallel slab model will lead to large deviations in the evaluation of the material migration characteristics in the rock mass, especially the intersection, and it is necessary to establish corrections for the geometric characteristics of the fractured intersection in future studies. Model to improve the accuracy of the assessment.**

## Keywords

**Three-dimension crossed fractures; Fluid flow behaviour; Solute transport behaviour; Navier-Stokes equation; Peclet number.**

## 1. Introduction

Solute transport in fractured media is an emerging research hotspot involving multidisciplinary cross-fusion. It has a high degree of complexity. Due to the randomness of the spatial distribution of fractures and the uncertainty of permeability parameters, the research on solute transport in fractured media has become extremely difficult. In 1953, Taylor[1] studied the transport of solutes in the fluid in a straight circular tube and deduced the expression of the diffusion coefficient. Aris[2] studied the situation in an elliptical tube and extended Taylor's research further. Detwiler, Rajaram and other scholars [3] have shown through experiments that Taylor dispersion and macroscopic dispersion will affect the process of solute transport in rough fissures.

Moreno [4] and Thompson [5] found through numerical simulations that the roughness of two-dimensional fractures can have an important impact on fluid flow and solute transport characteristics. Mourzenko et al. [6] studied two smooth intersecting fractures by particle tracking method. The results show that the Pe number plays an important role in the solute transport. When the Pe number tends to infinity, both the analytical model and the numerical model are close to the streamline path mode. Zou et al. [7] simulated the solute transport in the three-dimensional cross fissures, studied the

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relationship between the solute transport characteristics and the Pe number, and qualitatively evaluated the influence of the fissure roughness.

Most of the previous studies simplified the fractures as parallel flat plates, and a few studies that considered the roughness did not delve into the quantitative relationship between the roughness, fracture shear, and intersection morphology and seepage mass transfer characteristics. In response to the above problems, this study constructed a three-dimensional cross-fracture model considering the shear displacement to simulate the migration and mixing process of solutes in the three-dimensional cross-fracture. Influence of mixing characteristics.

## 2. Numerical modeling of 3D intersecting fractures

The surface morphology of the structural surface in the rock mass is rough and conforms to fractal distribution, so the fractal algorithm can be used to generate the rough surface of fracture by computer. Successive random increase method, which is has been widely applied in previous studies contribution to it is efficient and fast, as well as applied in this research.

In two-dimensional SRA, a single-valued continuous function $a(x,y)$ is used to describe the aperture of a rough fracture surface. The stationary increment of the function $a(x,y)$is defined as $[a(x+\Delta x, y+\Delta y)-a(x,y)]$, which obeys the Gaussian normal distribution with mean zero and variance $\sigma^2$ at distance $l\left(l=\sqrt{(\Delta x)^2+(\Delta y)^2}\right)$.The aperture of the self-affine surface defined by this function obeys the following rules:

$$\langle a(\mathrm{x}+\mathrm{r}\Delta\mathrm{x},\mathrm{y}+\mathrm{r}\Delta\mathrm{y})-\mathrm{a}(\mathrm{x},\mathrm{y})\rangle=0 \quad (1)$$

$$\sigma^2(r)=r^{2H}\sigma^2(1) \quad (2)$$

where,$\langle\cdot\rangle$ is the mathematical expectation; r is a constant; H is the Hurst exponent, ranging from 0 to 1; $\sigma^2$ is the variance that is defined as a function of $r$:

$$\sigma^2(r)=\langle[Z(x+r\Delta x,y+r\Delta y)-Z(x,y)]^2\rangle \quad (3)$$

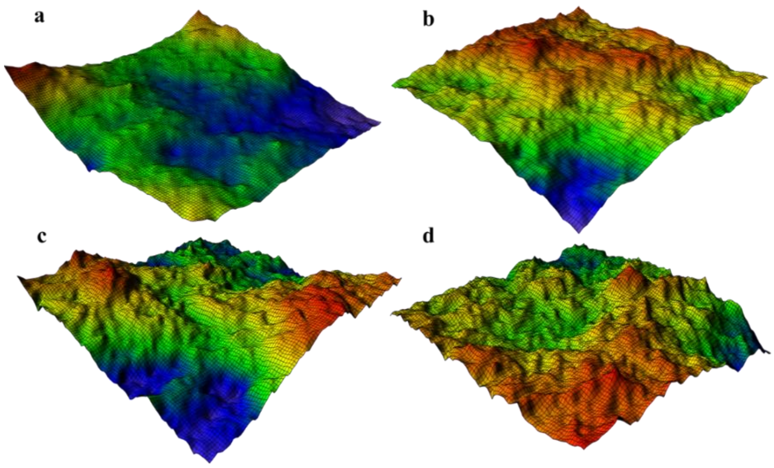


Fig. 1. Roughness fracture surface with different fractal dimension generated by SRA method: (a) D=2.55;(b) D=2.60; (c) D=2.65; (d) D=2.70.

In this study, a series of three-dimensional self-affine rough surfaces were constructed by SRA method, Fig.3 shows four fracture surfaces with 256 mm lengths and widths with numerical interpolation spacing 0.1mm, H indices are 0.3, 0.35, 0.4, 0.45, and corresponding fractal dimensions of 2.7, 2.65, 2.6, and 2.55 the bigger the H, the surface has more higher spatial correlation and smoother.

First, raise the fracture surface up by 1mm to form a fracture cavity with matched upper and lower surfaces, then move the upper surface 1 mm along the x direction to simulate fracture shear and form

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different aperture in fracture (as shown in Fig.2(b)). The upper and lower the fracture are denoted by U and D respectively, and both surfaces are divided into 4 symmetrical parts and coded, as shown in Figure 2(a). The established cross-fracture model with roughness surface is shown in Figure 2(c), the size of model in X, Y, and Z directions are 10 mm, 5 mm, and 10 mm, respectively. Since the permeability of the hard-rock is very low compared with that of the fracture, the diffusion of solute along the matrix is not considered. At the same time, the cross fissures with corresponding mechanical apertures are established as shown in Fig. 2(d).

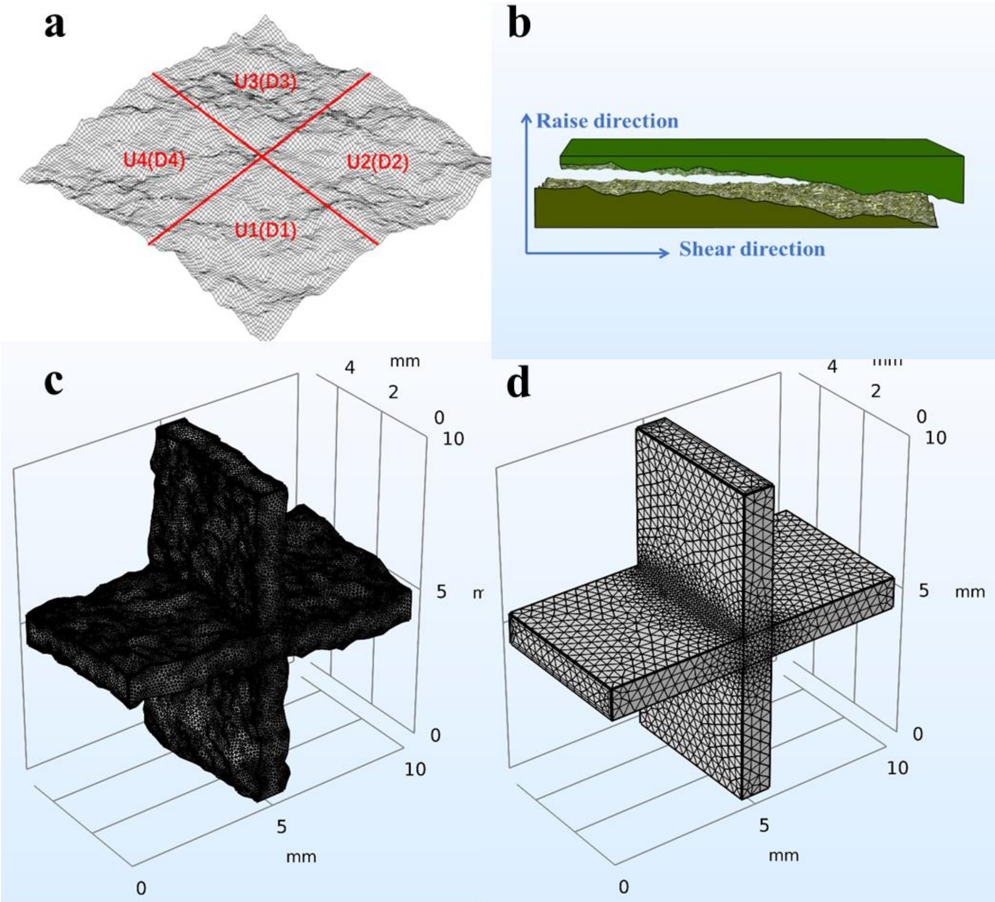


Figure.2 3D crossed rough-walled fracture model and parallel-plate model: (a) Schematic diagram of fracture surface division; (b) Schematic diagram of fracture shear; (c) Three-dimensional cross-rough fracture model; (d) Three-dimensional cross smooth fracture model.

## 3. Numerical method for simulation of seepage and solute transport in cross-fracture

In this study, COMSOL Multiphysics was used to solve the seepage flow and solute transport in the cross fracture, which realizes the simulation of real physical phenomena by solving partial differential equations (single physics field) or partial differential equations (multi physics field). The solution of the physical field governing equations in the model uses the fluid flow-laminar flow module (spf) and the chemical species transfer-transfer of dilute species (tds) module, of which the "Laminar Flow (spf)" module is used to solve the Navier-Stokes equations of conservation of momentum and the equations of conservation of mass; "Transport of Diluted Species (tds)" module is used to calculate the concentration field of dilute solutes.

### 3.1 Governing equation

Assuming that the fluid in fracture is isothermal and stable incompressible Newtonian fluid, the governing equation of seepage flow obey following Navier-Stokes equation:

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$$\nabla \cdot u = 0 \tag{4}$$

$$\rho u \cdot \nabla u - \mu \nabla^2 u = -\nabla P \tag{5}$$

In the formula: $\nabla^2$ is Laplace operator; $u$ is the flow velocity (m/s); $\rho$ is density of fluid (kg/m$^3$); $P$ is pressure (Pa); $\mu$ is dynamic viscosity (Pa·s). In this study, the solvent is water and the solute concentration is low. Solute transport conforms to Fick's first law. The governing equation can be written as:

$$u \cdot \nabla C - \nabla \cdot D(\nabla C) = 0 \tag{6}$$

where: $C$ is the solubility of the solute (kg/m$^3$); $D$ is diffusion coefficient (m$^2$/s).

### 3.2 Initial and boundary conditions

The two branch end faces are fluid inlets. In order to facilitate calculation and control of the Pe number, it is assumed that the flow rates at the two inlets are equal. Due to the different areas of the two inlets, a constant flow inlet boundary condition is used to ensure that the flow rates of the two inlets are equal. One inlet is pure water, and the other inlet is continuously injected a solution with a concentration of $C=C_0=1mol/m^3$. sections 3 and 4 are outlets, and the boundary conditions are set to pressure $P=0$. The fluid only flows inside the fracture, and the permeability of the surrounding matrix is negligible. Tracer breakthrough curves is a characteristic of fracture flow, which simulated usinga particle tracking technique. The transport properties for the different realizations are studied by comparing the mean residencetime and dispersion. The mean residencetime and variancemay be usedto determinethe Peclet number Pe, which is a dimensionless quantity calculated by the following formula[6]:

$$Pe = \frac{Q}{WD} \tag{7}$$

In the formula: $Q$ is the flow rate (m$^3$/s); $W$ is the width of the fracture (m). The Reynolds number is another important parameter to characterize fractured fluid, representing the state of fluid flow, following the formula:

$$Re = \frac{\rho Q}{W\mu} \tag{8}$$

Research by Johnson et al. showed that the Pe number in the range of 0.1 to 610 includes almost all types of solute transport processes. In nature, fluids generally flow in fractures at a relatively low speed. In order to ensure that the fluid in linear state, Re is less than 1 in this study. The parameters of the numerical model are shown in Table 1.

Table 1. Model parameter table

| parameter | Unit | Value |
|---|---|---|
| Fluid density | ρ/(Kg/m$^3$) | 999.7 |
| Dynamic viscosity | μ /(Pa·s) | $1.307\times10^{-3}$ |
| Gravity acceleration | g/(m/s$^2$) | 9.81 |
| Diffusion coefficient | D/(m$^2$/s) | $2.03\times10^{-9}$ |
| Inlet flow | Q/(m$^3$/s) | $2.030\times10^{-12}$, $2.030\times10^{-11}$, $2.030\times10^{-10}$, $1.015\times10^{-9}$, $2.030\times10^{-9}$, $4.060\times10^{-9}$, $1.015\times10^{-8}$, $1.238\ 3\times10^{-8}$ |
| Injection concentration | C0/(mol/m$^3$) | 0.2 |
| Petrley number | Pe/(1) | 0.1, 1, 10, 50, 100, 200,500, 610 |
| Reynolds number | Re/(1) | 0.000 2, 0.001 6, 0.015 5, 0.077 6, 0.155 3, 0.310 5, 0.776 4, 0.947 1 |

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# 4. Analysis of flow and solute transport in crossed fractures

## 4.1 Flow field analysis

Since the fluid is in a linear state and the flow fields under different Pe number conditions are consistent, only the calculation results under the conditions of Pe=1($Q=2.030\times10^{-11}m^3/s$) are used for analysis. The flow fields of the four surface roughness fracture models are shown in the fig 3.

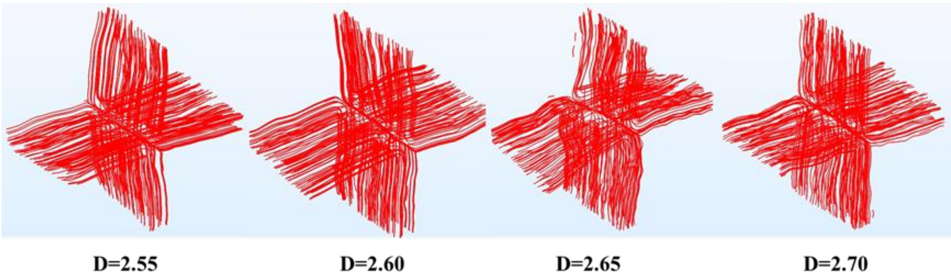
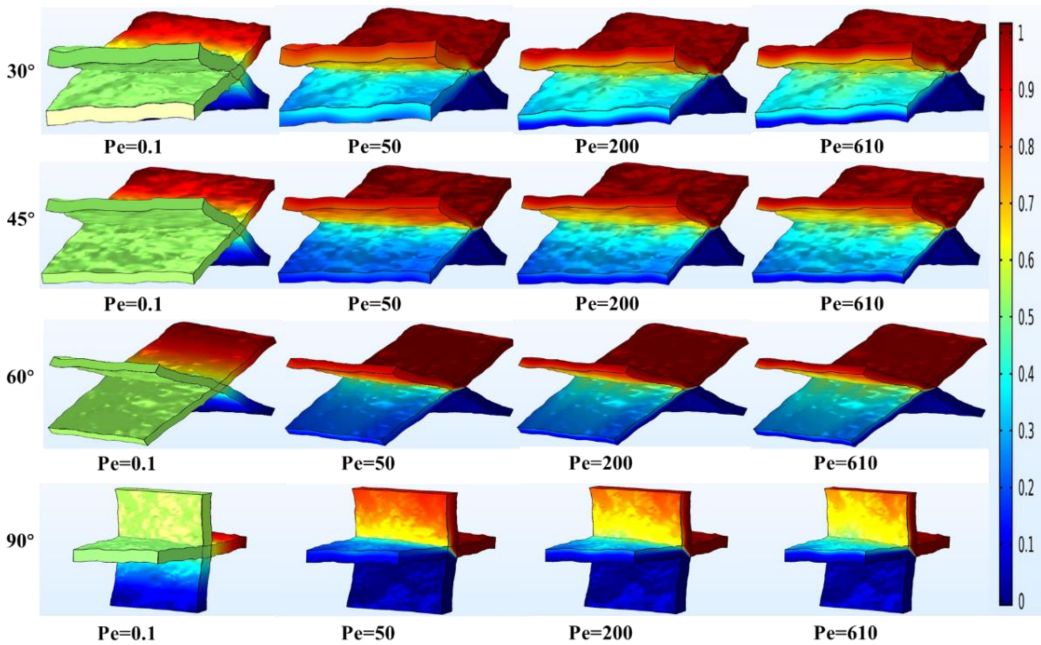



Fig. 3 Flow field distribution of different fracture surface fractal dimension when Pe=1

In the parallel plate model, the flow field distribution is uniform and symmetric. The fluids only flow in from one branch and flow out from one branch. They do not interfere with each other at the intersection, and there is no mixing situation, which conforms to the general movement of the fluid in the linear flow state. law. In the rough fracture model, the streamline is strongly curved in the fracture, and the flow fields of the four branches are asymmetrically distributed, and there is a phenomenon of channeling. The tortuosity of this streamline is caused by the heterogeneity of the cavity structure caused by the rough surface. And as the surface roughness of the crack increases, the unevenness of the flow becomes more obvious.

## 4.2 Solute distribution analysis

In order to analyze the influence of the fracture geometry on the solute transport in the intersecting fractures, the different surface fractal dimensions (D=2.55, 2.65, 2.70) of the fractures at different angles (30°, 45°, 60°, 90 °) when the solute transport is analyzed, Figure 4 shows the solute distribution in some cases.




(a) Concentration distribution diagram at different angles when D=2.55

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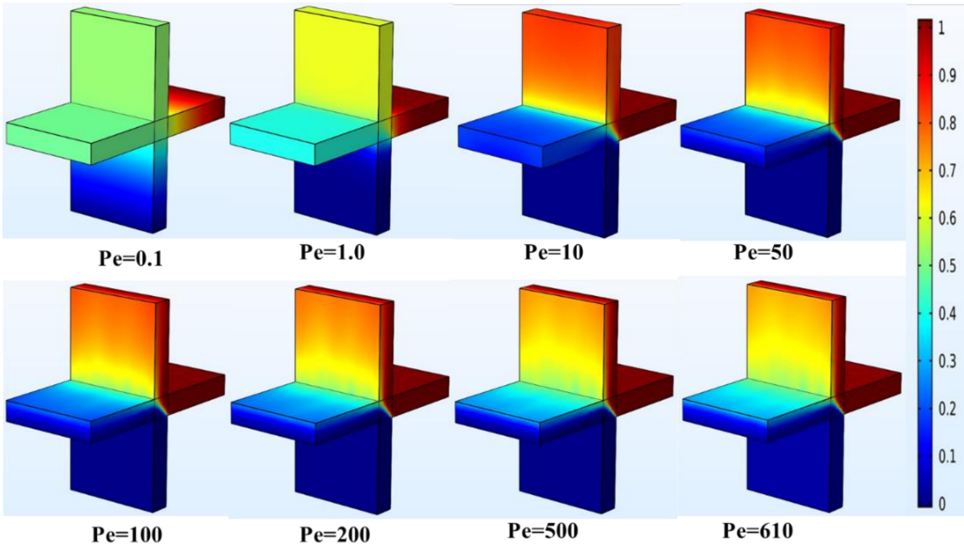
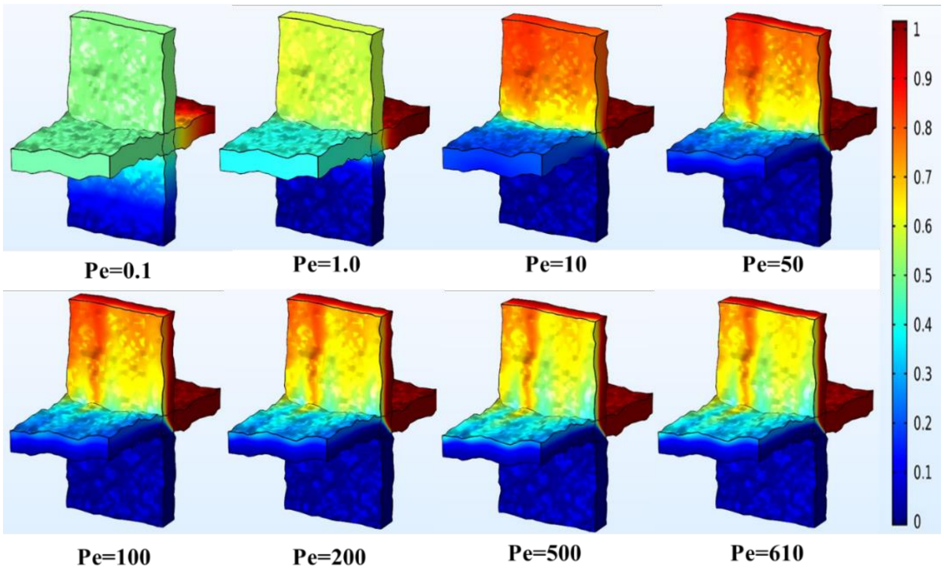



(b) Distribution of solute in crossing fractures of smooth plate at different Pe numbers




(c) Distribution of solute in crossing fractures with D=2.70 at different Pe numbers

Figure 4 Solute distribution diagram

It can be seen from the simulation results that when Pe=1, the dominant mode of solute migration in the fissure is diffusion, and the concentrations at the two outlets are uniformly distributed. As the number of Pe gradually increases, the mode of solute migration is also The solute diffusion begins to decrease, the convection part begins to increase, and the solute gradually gathers toward the outlet 4. When Pe>10, it can be clearly seen that the solute migration mode begins to change. When Pe>500, it can be Ignoring the diffusion of molecules, the dominant mode of solute migration in the intersecting fissures is convection. At this time, the up and down layering of the solution can be observed in the outlet branch. This layering phenomenon is due to the fluid from different inlets at the intersection of the fissure. It is caused by entering the exit branch in a stratified manner without mixing.

In order to quantitatively describe the solute transport characteristics of the cross fissure, this study uses the mixing ratio to describe the degree of solute mixing when passing through the cross fissure, which is defined as[8]:

$$M_r = \frac{Q_3 \cdot C_3}{Q_3 \cdot C_3 + Q_4 \cdot C_4} \tag{9}$$

where: $Q_3$ and $Q_4$ are the average flow rates of the two outlet fluids respectively; $C_3$, $C_4$ is the average concentration of the two outlet solutions. The mixing ratio is shown in Figure 5.

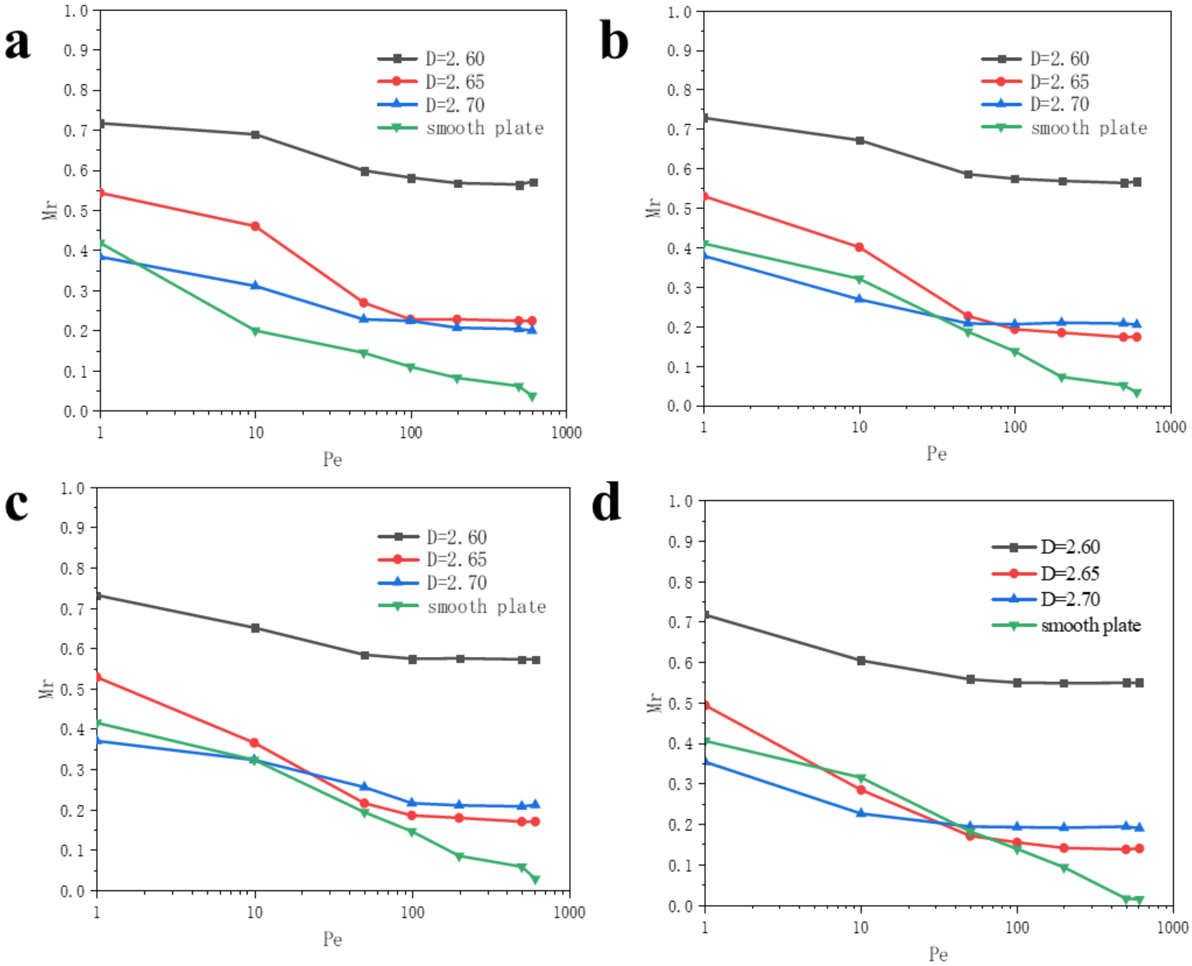



Fig.5 Variation of solute mixing ratio with Pe at different angles: (a) crossing angle of fractures is 30°; (b) crossing angle of fractures is 30°; (b) crossing angle of fractures is 60°; (b) crossing angle of fractures is 90°;

The different angles of the intersecting fissures will cause differences in solute mixing ability. When the number of Pe increases from 1 to 10, the mixing ratio of 60° in the three models of 30°, 45°, and 60° decreases the most, and the range of change is the most obvious. This is directly related to the phenomenon of channeling. The flow enhances the mixing of the fluid, so that the solute has more opportunities to enter the dominant channel. So that the model always maintains a high mixing ratio. As the number of Pe continues to increase, the mixing ratio of models from all angles continues to decrease, and the final mixing ratio remains at 0.2.

In general, with the increase of the Pe number, the changing trend of the model mixture ratio under the four angles is the same, and the decline is different. Compared with the flat plate without roughness, due to the roughness, when the Pe number is large enough, the solute does not only flow out from one outlet, but mostly flows out through the dominant channel, and a small part flows out from the other branch outlet. . Therefore, the final mixing ratio will not be the same as in the ideal state of the plate, tending to zero. It reflects the effect of roughness on solute mixing.

## 5. Conclusions

In this study, a three-dimensional cross-fracture model with a rough surface was generated, numerical simulations of seepage and solute transport were carried out, and the geometric morphology of the

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fracture surface and the concentration distribution and mixing law in the fracture under different Pekeley numbers were studied. The main conclusions as follows:

(1) In the rough fracture model, the heterogeneity of the geometry at the intersection leads to the channeling of the fluid, which promotes the mixing of solutes, resulting in a larger mixing ratio than the ideal model (parallel flat plate) and other rough models. The fluid tends to flow to the dominant channel, and the specific channeling position is closely related to the fracture geometry.

(2) The qualitative mixing behavior is closely related to the Pe number. Theoretically, as the number of Pe increases, the measured mixing ratio at the outlet generally gradually decreases from 0.5 and tends to zero. Due to the effect of channeling, the mixing ratio in this study has always maintained a value greater than 0.5, and the range of change is small, showing the controlling effect of the dominant seepage channel on the material transport characteristics.

(3) When the Pe number is 0.1~10, the migration of the solute is dominated by diffusion. At this time, the solute is completely mixed at the intersection; as the Pe number gradually increases, the mixing mode of the intersection gradually changes from the completely mixed mode to the streamline Path mode conversion; when the Pe number is greater than 50, the mixing ratio no longer changes. It can be considered that the transport of solutes is dominated by convection, which is at least one order of magnitude smaller than the theoretical critical value, showing the complex geometry of the intersection Appearance has a huge influence on the mixing behavior of solutes.

(4) The intersection angle of the intersecting fissures will also affect the solute transport process. In this study, The four angle models of 30°, 45°, 60°, and 90° are selected. The study found that in the same roughness and the same Pe number, the mixing ratio at 30° is the largest. As the angle increases, the mixing ratio decreases. small.

Natural fracture in nature have complex surface features. At the same time, due to the influence of natural stress and man-made disturbances, a large number of fractures produce shear deformation, which significantly changes the geometric characteristics and mechanical, seepage, and material migration characteristics of the cracks. The results of this paper reconfirm the huge errors that may be caused by the classical parallel plate model, and quantitatively evaluate the significant influence of fluid channeling on solute transport caused by the heterogeneity of the geometric morphology of the cross fracture, which has a significant impact on the related engineering construction. It has guiding significance and is an important supplement to existing research.

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